The Vinylogous Reactivity of Oxindoles Bearing Nonsymmetric 3-Alkylidene Groups

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Study of the double bond isomerization of oxindole (*E*)-**1a** and (*Z*)-**1a**

Table S1. Isomerization experiment of oxindoles (*Z*)-**1a** and (*E*)-**1a** with catalyst **I**.^a

$\xrightleftharpoons[\text{Tol 0.1 M, 25 } ^\circ\text{C}]{\text{I, (20 mol \%)}}$

entry	catalyst	t (h)	(<i>Z</i>)- 1a :(<i>E</i>)- 1a ^b
1	I	0	100:0
2	I	48	66:34
3	I	0	0:100
4	I	48	66:34

^aUnless otherwise noted, all reactions were performed using 0.2 mmol of (*Z*)-**1a** or (*E*)-**1a**, 20 mol % of **I** and 2 ml of toluene.

^bDetermined by ¹H NMR of the crude mixture.

Two experiments were performed in which the two isolated oxindoles (*E*)-**1a** and (*Z*)-**1a** were placed separately under reaction conditions for 48 h to check the stability of the double bond. In both cases we observed that the geometry of the double bond was unstable and an equilibrium mixture of 66 : 34 of (*Z*)-**1a** : (*E*)-**1a** was obtained.

Figure S1: Upper spectrum reaction mixture after isomerization. Bottom spectrum pure oxindole (*E*)-**1a**

NDI_024_Z_pulito_H

Sample: DC061 rid_frazioneB_c

File: home/rosini/vnmrsws/data/NDI/NDI_024_Z_pulito_H.fid

Pulse Sequence: s2pul

Figure S2: Upper spectrum reaction mixture after isomerization. Bottom spectrum pure oxindole (Z)-1a

Isomerization reaction of (Z)-4a to (E)-4a at different temperature

In the reaction of oxindole (E)-1a together with the desired product (Z)-4a traces of the product of isomerization (E)-4a were detected. We confirmed that (Z)-4a when treated with **I** (20 mol %) at -20 °C in toluene isomerizes to (E)-4a with an equilibrium ratio of 95:5 after 72 hours.

Table S2: Isomerization of (Z)-4a to (E)-4a.

Entry	Temperature	(Z)-4a:(E)-4a
1	25 °C	91:9
2	0 °C	92:8
3	-20 °C	95:5

Synthesis of methyl (E)-2-((tert-butyldimethylsilyl)oxy)-3-(pent-2-en-3-yl)-1H-indene-1-carboxylate (**10**)

The title compound was obtained from the corresponding non-silylated oxindole **1g** after treatment with 1.25 eq. of *tert*-butyldimethylsilyl trifluoromethanesulfonate and 1.4 eq. of triethylamine in DCM (0.25 M) for 96 hours. After this time the crude mixture was concentrated and flash chromatography (hexane/ethyl acetate 9/1) afforded the pure product as the single (*E*)-isomer in 86% yield. It is crucial for the reaction to be efficient to handle the starting triflate carefully, in fact when the reaction was performed with a dated reagent the yield dramatically decreased.

¹H NMR of **10** (400 MHz, CDCl₃): δ (ppm): 8.01 (*m*, 1H); 7.42 (*m*, 1H); 7.18 (*m*, 2H); 5.64 (*q*, 1H, *J*₁ = 6.9 Hz). 3.98 (*s*, 3H); 2.44 (*q*, 2H, *J*₁ = 7.5 Hz); 1.82 (*d*, 3H, *J*₁ = 6.9 Hz); 1.01 (*s*, 9H); 0.90 (*t*, 3H, *J*₁ = 7.5 Hz); 0.13 (*s*, 6H).

NDI_232_96h_H

Sample: NDI_232_96h_H

File: home/rosini/vnmrsws/data/NDI/NDI_232_96h_H.fid

Pulse Sequence: s2pul

Irradiated protons

Vicinal protons

Experimental evidences for the reaction of the *s-trans* intermediates in the vinylogous reactions of oxindoles with nitroalkenes.

The protocols presented by Casiraghi and Wang were limited to oxindoles having a single vinylogous or at least two equivalent vinylogous γ and γ' sites of reaction.

Even if the presence of an *s-cis* enolate as the only intermediate of reaction was advanced by both research groups no concrete explanation based on rational mechanism approach was given for the site selectivity observed. In particular with 3-alkylidene oxindole **A** having methyl groups at the γ and γ' positions it is not possible to exclude that the *s-trans* enolate intermediate reacts to give the observed Michael adduct (scheme S1).

Scheme S1: Possible reaction path where both *s-cis* and *s-trans* enolates react to give the same product.

Both enolates could add the same enantiotopic *Si*-face of nitroalkene and furnish the same product with the same absolute configuration of the chiral center. Obviously in the case the *s-trans* intermediate, the most stable (*Z*)-configured Michael adduct, will be obtained only after equilibration, mediated by the catalyst, of the (*E*)-adduct. This hypothesis is supported mainly by various experimental data. First of all when (*Z*)-2-oxo-3-(1-phenylethylidene)indoline-1-carboxylate **B** was used the (*E*)-Michael adduct is obtained. This result can be admitted only if oxindole **B** isomerizes to the corresponding (*E*)-isomer **B'** and reacts via *s-cis* enolate to give the vinylogous product (scheme S2a). However oxindole **B** does not isomerize during the reaction condition as we readily observed (scheme S2b) thus indicating that the *s-trans* intermediate can be formed and reacted to furnish the (*Z*)-product and finally isomerize to the most stable (*E*)-isomer.

Scheme S2: vinylogous reaction of **B** oxindole and experiments of isomerization.

To demonstrate this hypothesis we performed two separate reactions using our optimized conditions with oxindole **B** and **B'**. Oxindole **B** reacted very quickly giving an almost quantitative conversion of the (*E*)-Michael adduct in 23 hours at -20 °C using 20 mol% of catalyst loading together with traces of the (*Z*)-Michael adduct (table S3). This result shows that the (*Z*)-Michael adduct isomerize, probably with the action of the catalyst to the more stable (*E*)-Michael adduct. Oxindole **B'** is less reactive under the same conditions and gave only a 12% of conversion after 23 hours in the corresponding (*E*)-Michael adduct via *s-cis* enolate intermediate (table S4).

Table S3: vinylogous reaction of **B** oxindole.

Oxindole	Time [h]	Conversion [%]
B	1	15
	3	65
	5	73
	23	91

Table S4: vinylogous reaction of **B'** oxindole.

Oxindole	Time [h]	Conversion [%]
B'	1	2
	3	5
	5	7
	23	12

This results outlined that the γ -position is probably less reactive than the γ' in the case of type **B** oxindoles, thus with high probability the *s-trans* enolate is the reactive intermediate of the reaction. This results could not be directly applied to oxindole **A** because they are different substrates and could have different reactivity. However they are representative for the complexity of the reaction mechanism of the vinylogous reaction of oxindoles.

Conformational analysis and absolute configuration determination of (Z)-**4n**

All the attempts to obtain good single crystals of the compounds belonging to the (Z)-**4x** series were not successful, for this reason it was not possible to assign the absolute configuration by the anomalous dispersion X-ray method.¹ For this reason the relative and absolute configuration were determined by a combination of conformational analysis and theoretical simulations of chiro-optical spectra. Compound **6** was selected as representative compound.

The geometry of the double bond was preliminary determined by NOE-NMR, that confirmed the Z configuration. On saturation of the allylic CH₂, a strong NOE was observed on the H-4 of the oxindole. The determination of the absolute configuration (AC) of chiral molecules using chiro-optical techniques like optical rotation (OR), electronic circular dichroism (ECD), and vibrational

circular dichroism (VCD) has gained feasibility and reliability because of the development of methods for the prediction of these properties based on density functional theory (DFT) and on its Time-Dependent formalism (TD-DFT).² As a first attempt the theoretical calculation of the electronic circular dichroism spectra (ECD) was selected for the absolute configuration assignment. As the first stage, we performed a conformational search on a model compound where the propyl moiety was reduced to a methyl group (model compound **6**). This approach lowers the

conformational space to be explored at a great extent, while preserving all the acting UV chromophores. All the conformations found by MM search within a 10 kcal/mol window (Monte Carlo searching together with the MMFF94 molecular mechanics force field as implemented in Titan 1.0.5, Wavefunction inc.) were then optimized using DFT at the B3LYP/6-311++G(2d,p) level³. The harmonic vibrational frequencies of each conformation were calculated at the same level to confirm their stability (no imaginary frequencies were observed) and to evaluate the enthalpy and Gibbs free energy of each conformation (Table S5).

Table S5: Relative energies of the four conformations (**a-d** as from Figure S1). Calculations at the B3LYP/6-311++G(2d,p) level.

Conformer	E (kcal/mol)	H° (kcal/mol)	G° (kcal/mol)
a	0.00	0.00	0.21
b	0.15	0.16	1.21
c	0.38	0.36	0.00
d	0.63	0.62	0.82

After DFT minimization four conformations were found to be clustered in a narrow energy window (see Figure S3). These conformations (**a**, **b**, **c**, **d**) differ because of the different dihedral angles 1-2-3-4 (**a**, **b**) and 2-3-4-5 (**c**, **d**).

Figure S3. 3D view of the four most stable conformations of **6**, calculated at the B3LYP/6-311++G(2d,p) level.

The electronic excitation energies and rotational strengths have been calculated for the isolated molecule in the gas phase for the best conformations of **6**, using TD-DFT with four different methods (functionals), to ascertain if different computational approaches provide different shapes of the simulated spectra.⁴ Simulations were performed with the hybrid functionals BH&HLYP⁵ and M06-2X,⁶ the Long-range Correlated ω B97XD that includes empirical dispersion,⁷ and CAM-B3LYP that includes long range correction using the Coulomb Attenuating Method.⁸ The calculations employed the same 6-311++G(2d,p) basis set that proved to be sufficiently accurate at a reasonable computational cost.⁹ Rotational strengths were calculated in both length and velocity representation, the resulting values being very similar (RMS differences < 5%). For this reason the errors due to basis set incompleteness should be very small, or negligible.¹⁰

All the calculations were performed supposing 4'R absolute configuration, with the results shown in Figure S4. The simulated spectra of the separated conformations show very different trends, probably because of the high conformational freedom of the carbon chain, which yields conformations with different spatial relationship between the chromophores.

Figure S4. TD-DFT simulated spectra calculated for **6** using four different functionals (CAM-B3LYP, BH&HLYP, ω B97-XD, M06-2X) and the same basis set 6-311++(2d,p). For each conformation the first 50 excited states were calculated and the spectrum was obtained using a 0.15 eV line width at half height.

Given the different trend of the components, the shape of the simulated spectrum to be compared with the experimental one will strongly depend on the population ratio employed. Unfortunately, because of the low steric hindrance to rotation about the sp^3 - sp^3 bonds, the experimental population distribution of all conformations could not be detected by low temperature NMR¹¹. The evaluation of the population ratio was evaluated with the Boltzmann distribution based on the calculated ground state internal energies and the resulting spectra are shown in Figure S5.

Figure S5. Simulations of the experimental ECD spectrum of (Z)-**4n** (black traces). For each section, the black line correspond to the experimental spectrum (acetonitrile solution, 5×10^{-5} M, 0.2 cm path length, $\Delta\epsilon$ in $\text{Mol L}^{-1} \text{cm}^{-1}$). The simulated spectra were vertically scaled and shifted from -6 to 4 nm to get the best match with the experimental spectrum.

All the four simulations obtained display a nice agreement with the experimental spectrum and the best simulation is the one obtained with the BH&HLYP functional. The 4'*R* absolute configuration could be therefore assigned to (Z)-**4n**. However the experimental trace is rather weak and the ECD simulation could be not fully reliable.

To have another and independent assignment of the absolute configuration we investigated the optical rotation data. Compound (Z)-**4n** was prepared following the procedure reported by Casiraghi and co-authors,¹² where the absolute configuration of (4'*R*)-(Z)-6-chloro-1-methoxycarbonyl-3-(5-nitro-4-phenylpentan-2-ylidene)indolin-2-one (analogue to the model compound **6**) has been determined by the Anomalous Dispersion X-Ray method. Thus it is likely to compare the $[\alpha]_D^{20}$ sign of (Z)-**4n** with that reported for **6**. According to the sign of the and the same priority of the substituents at the stereogenic centre, we can assign *R* absolute configuration (figure S6).

Figure S6. Left: Optical rotation of the reported compound **6** (solution 1.0 g 100 mL⁻¹ in CHCl₃, 10 cm cell length, 1 mL capacity, $[\alpha]_D^{20}$ in units of 10 deg cm² g⁻¹). Right: Optical rotation for of (Z)-**4n** (solution 1.0 g 100 mL⁻¹ in CHCl₃, 10 cm cell length, 1 mL capacity, $[\alpha]_D^{20}$ in units of 10 deg cm² g⁻¹).

A further confirmation of the assigned absolute configuration was given by the comparison between the experimental ECD spectra, recorded for **6** (prepared by our group) and for (Z)-**4n**. As from Figure S7, the two spectra have similar trend, having positive and negative Cotton effects at the same wavelengths. In particular they have a relevant negative Cotton effect at 301 nm and a positive effect at 265 nm.

Figure S7. Experimental ECD spectra for **6** and (Z)-**4n**. The blue line corresponds to compound **6** (acetonitrile solution, 5x10⁻⁵M, 0.2 cm path length, $\Delta\epsilon$ in Mol L⁻¹ cm⁻¹), the red line is for (Z)-**4n** (acetonitrile solution, 5x10⁻⁵M, 0.2 cm path length, $\Delta\epsilon$ in Mol L⁻¹ cm⁻¹).

Conformational analysis and absolute configuration determination of (Z)-3h

Good crystals suitable for X-ray diffraction were obtained for compound (Z)-**3h** by slow evaporation of a *n*-hexane/isopropanol solution. The anomalous scattering determination of the absolute configuration was possible thanks to the presence of the bromine atom. The 3*Z*,3'*R*,4'*R* configuration was determined for the selected crystal. This assignment further confirmed the 4'*R* absolute configuration of (Z)-**4o**.

Figure S8. X-Ray structure of (Z)-3h.

Crystal Data for compound (Z)-3h

Molecular formula: $\text{C}_{23}\text{H}_{23}\text{N}_2\text{O}_5\text{Br} \cdot 1/2 \text{ H}_2\text{O}$, $M_r = 496.35$, monoclinic, space group C_2 , $a = 15.584(2)$, $b = 12.3431(19)$, $c = 13.574(2) \text{ \AA}$, $\beta = 121.3460(10)$ $V = 2229.8(6) \text{ \AA}^3$, $T = 298(2) \text{ K}$, $Z = 4$, $\rho_c = 1.479 \text{ g cm}^{-3}$, $F(000) = 1020$, graphite-monochromated $\text{MoK}\alpha$ radiation ($\lambda = 0.71073 \text{ \AA}$), $\mu(\text{MoK}\alpha) = 1.883 \text{ mm}^{-1}$, colourless brick ($0.40 \times 0.35 \times 0.15 \text{ mm}^3$), empirical absorption correction with SADABS (transmission factors: $0.7654 - 0.5196$), 2400 frames, exposure time 20 s, $1.76 \leq \theta \leq$

27.00, $-19 \leq h \leq 19$, $-15 \leq k \leq 15$, $-17 \leq l \leq 17$, 12500 reflections collected, 4821 independent reflections ($R_{\text{int}} = 0.0309$), solution by direct methods (SHELXS97) and subsequent Fourier syntheses, full-matrix least-squares on F_o^2 (SHELXTL 6.10), hydrogen atoms refined with a riding model, data / restraints / parameters = 4821 / 1 / 291, $S(F^2) = 1.048$, $R(F) = 0.0402$ and $wR(F^2) = 0.0929$ on all data, $R(F) = 0.0356$ and $wR(F^2) = 0.901$ for 4363 reflections with $I > 4\sigma(I)$, weighting scheme $w = 1/[\sigma^2(F_o^2) + (0.0501P)^2 + 0.000P]$ where $P = (F_o^2 + 2F_c^2)/3$, largest difference peak and hole 0.297 and $-0.328 \text{ e } \text{\AA}^{-3}$. Flack parameter ^a for R,R configuration: $-0.006(7)$. The crystal cell contains a molecule of water in a special position. Crystallographic data (excluding structure factors) for the structure reported in this paper have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication no. CCDC-1015561. Copies of the data can be obtained free of charge on application to CCDC, 12 Union Road, Cambridge CB21EZ, UK (fax: (+44) 1223-336-033; e-mail: deposit@ccdc.cam.ac.uk).

^a Flack, H. D. *Acta Cryst.* **1983**, *A39*, 876-881

NOE experiments and NMR traces for starting oxindoles

NDI_024_pulito_E_H

Sample: NDI_024_pulito_E_H

File: home/rosini/vnmrsws/data/NDI/NDI_024_pulito_E_H.fid

Pulse Sequence: s2pul

NDI_024_E_pulito_C

Sample: NDI_024_E_pulito_C

File: xp

Pulse Sequence: s2pul

Solvent: cdcl3

Temp. 25.0 C / 298.1 K

Operator: rosini

Mercury-400BB "m400"

Relax. delay 2.000 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 24154.6 Hz

192 repetitions

OBSERVE C13, 100.5611202 MHz

DECOUPLE H1, 399.9265566 MHz

Power 41 dB

continuously on

WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 4 hr, 42 min, 47 sec

NDI_024_Z_pulito_H
 Sample: NDI_024_Z_pulito_H
 File: home/rosini/vnmrsys/data/NDI/NDI_024_Z_pulito_H.fid
 Pulse Sequence: s2pul

NDI_024_Z_pulito_C
 File: home/rosini/vnmrsys/data/NDI/NDI_024_Z_pulito_C.fid
 Pulse Sequence: s2pul

NDI_023_E_pulito_H

Sample: DCDC062g_h

File: home/rosini/vnmrsys/data/NDI/NDI_023_E_pulito_H.fid

Pulse Sequence: s2pul

NDI_023_E_pulito_C

Sample: NDI_023_E_pulito_C

File: xp

Pulse Sequence: s2pul

NDI_022_primamacchia_Z_H
 Sample: DC057_dosaggio_A3_h
 File: home/rosini/vnmrsys/data/NDI/NDI_022_primamacchia_Z_H.fid
 Pulse Sequence: s2pul

NDI_022_Z_pulito_C
 Sample: NDI_022_Z_pulito_C
 File: xp
 Pulse Sequence: s2pul

NDI_130_E_pulito_H

Sample: NDI_130_E_pulito_H

File: home/rosini/vnmrsys/data/NDI/NDI_130_E_pulito_H.fid

Pulse Sequence: s2pul

NDI_130_E_pulito_C

Sample: NDI_130_E_pulito_C

File: home/rosini/vnmrsys/data/NDI/NDI_130_E_pulito_C.fid

Pulse Sequence: s2pul

NDI_130_Z_pulito_H

Sample: NDI_130_Z_pulito_H
File: home/rosini/vnmrsys/data/NDI/NDI_130_Z_pulito_H.fid
Pulse Sequence: s2pul

NDI_130_Z_pulito_C

Sample: NDI_130_Z_pulito_C
File: home/rosini/vnmrsys/data/NDI/NDI_130_Z_pulito_C.fid
Pulse Sequence: s2pul

NDI_134_E_pulito_H

Sample: NDI_134_E_pulito_H
File: home/rosini/vnmrsys/data/NDI/NDI_134_E_pulito_H.fid
Pulse Sequence: s2pul

NDI_134_E_pulito_C

Sample: NDI_134_E_pulito_C
File: xp
Pulse Sequence: s2pul

NDI_134_Z_pulito_H

Sample: NDI_134

File: home/rosini/vnmrsys/data/NDI/NDI_134_Z_pulito_H.fid

Pulse Sequence: s2pul

NDI_134_Z_pulito_C

Sample: NDI_134_Z_pulito_C

File: home/rosini/vnmrsys/data/NDI/NDI_134_Z_pulito_C.fid

Pulse Sequence: s2pul

NDI_133_E_pulito_H

Sample: NDI_133_E_pulito_H
File: home/rosini/vnmrsys/data/NDI_133_E_pulito_H.fid
Pulse Sequence: s2pul

NDI_133_E_pulito_C

Sample: NDI_133_E_pulito_C
File: xp

Pulse Sequence: s2pul

Solvent: cdcl3
Temp: 25.0 C / 298.1 K
Operator: rosini
Mercury-400BB "m400"

Relax. delay 2.000 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 24154.6 Hz
304 repetitions
OBSERVE C13, 100.5611225 MHz
DECOUPLE H1, 399.9265566 MHz
Power 41 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 4 hr, 58 min, 7 sec

NDI_133_Z_pulito_H

Sample: NDI_133

File: home/rosini/vnmrsws/data/NDI/NDI_133_Z_pulito_H.fid

Pulse Sequence: s2pul

NDI_133_Z_pulito_C

Sample: NDI_133_Z_pulito_C

File: xp

Pulse Sequence: s2pul

NOE experiments for the determination of the geometry of the double bond for compounds (Z)-4a and (Z)-3a

NDI_028_A_H

Sample: NDI_027_B_H

File: home/rosini/vnmrsys/data/NDI/NDI_028_A_H.fid

Pulse Sequence: s2pul

NDI_027_B_H

Sample: NDI_027_B_H

File: home/rosini/vnmrsys/data/NDI/NDI_027_B_H.fid

Pulse Sequence: s2pul

NMR traces for Michael adducts

NDI_027_B_H

Sample: NDI_026_B_H

File: home/rosini/vnmrsys/data/NDI/NDI_027_B_H.fid

Pulse Sequence: s2pul

NDI_027_B_C

Sample: NDI_026_B_C

File: home/rosini/vnmrsys/data/NDI/NDI_027_B_C.fid

Pulse Sequence: s2pul

NDI_127_pulito_H
 Sample: NDI_127_pulito_H
 File: home/rosini/vnmrsys/data/NDI/NDI_127_pulito_H.fid
 Pulse Sequence: s2pul

NDI_127_pulito_C
 Sample: NDI_127_pulito_C
 File: home/rosini/vnmrsys/data/NDI/NDI_127_pulito_C.fid
 Pulse Sequence: s2pul

NDI_035_B_H

Sample: NDI_035_B_H

File: home/rosini/vnmrsys/data/NDI/NDI_035_B_H.fid

Pulse Sequence: s2pul

NDI_035_B_C

Sample: NDI_035_B_C

File: home/rosini/vnmrsys/data/NDI/NDI_035_B_C.fid

Pulse Sequence: s2pul

NDI_029_B_H

Sample: NDI_029_B_H

File: home/rosini/vnmrsys/data/NDI/NDI_029_B_H.fid

Pulse Sequence: s2pul

NDI_029_B_C

Sample: NDI_029_B_C

File: home/rosini/vnmrsys/data/NDI/NDI_029_B_C.fid

Pulse Sequence: s2pul

NDI_031_B_H

Sample: NDI_031_B_H

File: home/rosini/vnmrsws/data/NDI/NDI_031_B_H.fid

Pulse Sequence: s2pul

NDI_031_B_C

Sample: NDI_031_B_C

File: home/rosini/vnmrsws/data/NDI/NDI_031_B_C.fid

Pulse Sequence: s2pul

NDI_041_pulito_H

Sample: NDI_041_pulito_H

File: home/rosini/vnmrsys/data/NDI/NDI_041_B_H.fid

Pulse Sequence: s2pul

NDI_041_B_C

Sample: NDI_041_B_C

File: home/rosini/vnmrsys/data/NDI/NDI_041_B_C.fid

Pulse Sequence: s2pul

```
Sample: NDI_039_B_H
File: home/rosini/vnmrsys/data/NDI/NDI_039_B_H.fid
Pulse Sequence: s2pul
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```
Sample: NDI_039_B_C
File: home/rosini/vnmrsys/data/NDI/NDI_039_B_C.fid
Pulse Sequence: s2pul
```

NDI_039_pulito_F

Sample: NDI_039_pulito_F

File: home/rosini/vnmrsys/data/NDI/NDI_039_pulito_F.fid

Pulse Sequence: s2pul

NDI_037_B_H

Sample: NDI_037_B_H

File: home/rosini/vnmrsws/data/NDI/NDI_037_B_H.fid

Pulse Sequence: s2pul

NDI_037_B_C

Sample: NDI_037_B_C

File: home/rosini/vnmrsws/data/NDI/NDI_037_B_C.fid

Pulse Sequence: s2pul

NDI_180_pulito_H

Sample: NDI_180_pulito_H

File: home/rosini/vnmrsys/data/NDI/NDI_180_pulito_H.fid

Pulse Sequence: s2pul

NDI_180_pulito_C

Sample: NDI_180_pulito_C

File: xp

Pulse Sequence: s2pul

NDI_136_pulito_H

Sample: NDI_136_pulito_H

File: home/rosini/vnmrsys/data/NDI/NDI_136_pulito_H.fid

Pulse Sequence: s2pul

NDI_136_pulito_C

Sample: NDI_136_pulito_C

File: home/rosini/vnmrsys/data/NDI/NDI_136_pulito_C.fid

Pulse Sequence: s2pul

NDI_139_pulito_H

Sample: NDI_139_pulito_H

File: home/rosini/vnmrsys/data/NDI/NDI_139_pulito_H.fid

Pulse Sequence: s2pul

NDI_139_pulito_C

Sample: NDI_139_pulito_C

File: home/rosini/vnmrsys/data/NDI/NDI_139_pulito_C.fid

Pulse Sequence: s2pul

```
Sample: NDI_144_pulito_H
File: home/rosini/vnmrsys/data/NDI/NDI_144_pulito_H.fid

Pulse Sequence: s2pul
```

```
Sample: NDI_144_pulito_C
File: home/rosini/vnmrsys/data/NDI/NDI_144_pulito_C.fid

Pulse Sequence: s2pul
```

NDI_028_A_H

Sample: NDI_027_B_H

File: home/rosini/vnmrsws/data/NDI/NDI_028_A_H.fid

Pulse Sequence: s2pul

NDI_028_A_C

Sample: NDI_027_B_C

File: home/rosini/vnmrsws/data/NDI/NDI_028_A_C.fid

Pulse Sequence: s2pul

NDI_125_pulito_H
 Sample: NDI_125_pulito_H
 File: home/rosini/vnmrsys/data/NDI/NDI_125_pulito_H.fid
 Pulse Sequence: s2pul

NDI_125_pulito_C
 Sample: NDI_125_pulito_C
 File: home/rosini/vnmrsys/data/NDI/NDI_125_pulito_C.fid
 Pulse Sequence: s2pul

NDI_097_pulito_H

Sample: NDI_097_pulito_H

File: home/rosini/vnmrsys/data/NDI/NDI_097_pulito_H.fid

Pulse Sequence: s2pul

NDI_097_pulito_C

Sample: NDI_097_pulito_C

File: home/rosini/vnmrsys/data/NDI/NDI_097_pulito_C.fid

Pulse Sequence: s2pul

NDI_099_pulito_H

Sample: NDI_099_pulito_H

File: home/rosini/vnmrsys/data/NDI/NDI_099_pulito_H.fid

Pulse Sequence: s2pul

NDI_099_pulito_C

Sample: NDI_099_pulito_C

File: home/rosini/vnmrsys/data/NDI/NDI_099_pulito_C.fid

Pulse Sequence: s2pul

NDI_109_pulito_H

Sample: NDI_109_pulito_H

File: home/rosini/vnmrsys/data/NDI/NDI_109_pulito_H.fid

Pulse Sequence: s2pul

NDI_109_pulito_C

Sample: NDI_109_pulito_C

File: home/rosini/vnmrsys/data/NDI/NDI_109_pulito_C.fid

Pulse Sequence: s2pul

NDI_095_pulito_H

Sample: NDI_095_pulito_H

File: home/rosini/vnmrsys/data/NDI/NDI_101_pulito_H.fid

Pulse Sequence: s2pul

NDI_095_pulito_C

Sample: NDI_095_pulito_C

File: home/rosini/vnmrsys/data/NDI/NDI_101_pulito_C.fid

Pulse Sequence: s2pul

NDI_111_pulito_H

Sample: NDI_111_pulito_H

File: home/rosini/vnmrsys/data/NDI/NDI_111_pulito_H.fid

Pulse Sequence: s2pul

NDI_111_pulito_C

Sample: NDI_111_pulito_C

File: home/rosini/vnmrsys/data/NDI/NDI_111_pulito_C.fid

Pulse Sequence: s2pul

NDI_111_pulito_F

Sample: NDI_111_pulito_F

File: home/rosini/vnmrsys/data/NDI/NDI_111_pulito_F.fid

Pulse Sequence: s2pul

NDI_095_pulito_H

Sample: NDI_095_pulito_H

File: home/rosini/vnmrsys/data/NDI/NDI_095_pulito_H.fid

Pulse Sequence: s2pul

NDI_095_pulito_C

Sample: NDI_095_pulito_C

File: home/rosini/vnmrsys/data/NDI/NDI_095_pulito_C.fid

Pulse Sequence: s2pul

```
Sample: NDI_113_pulito_H
File: home/rosini/vnmrsys/data/NDI/NDI_113_pulito_H.fid

Pulse Sequence: s2pul
```

```
Sample: NDI_113_pulito_C
File: home/rosini/vnmrSYS/data/NDI/NDI_113_pulito_C.fid

Pulse Sequence: s2pul
```

NDI_178_pulito_H

Sample: NDI_178_pulito_H

File: home/rosini/vnmrsys/data/NDI/NDI_178_pulito_H.fid

Pulse Sequence: s2pul

NDI_178_pulito_C

Sample: NDI_178_pulito_C

File: xp

Pulse Sequence: s2pul

NDI_137_pulito_H

Sample: NDI_137_pulito_H

File: home/rosini/vnmrsys/data/NDI/NDI_137_pulito_H.fid

Pulse Sequence: s2pul

NDI_137_pulito_C

Sample: NDI_137_pulito_C

File: home/rosini/vnmrsys/data/NDI/NDI_137_pulito_C.fid

Pulse Sequence: s2pul

NDI_140_pulito_H
 Sample: NDI_140_pulito_H
 File: home/rosini/vnmrsys/data/NDI/NDI_139_pulito_H.fid
 Pulse Sequence: s2pul

NDI_140_pulito_C
 Sample: NDI_140_pulito_C
 File: home/rosini/vnmrsys/data/NDI/NDI_139_pulito_C.fid
 Pulse Sequence: s2pul

NDI_145_pulito_H

Sample: NDI_145_pulito_H

File: home/rosini/vnmrsys/data/NDI/NDI_145_pulito_H.fid

Pulse Sequence: s2pul

NDI_145_pulito_C

Sample: NDI_145_pulito_C

File: home/rosini/vnmrsys/data/NDI/NDI_145_pulito_C.fid

Pulse Sequence: s2pul

NDI_176_pulito_H

Sample: NDI_176_pulito_H

File: home/rosini/vnmrsys/data/NDI/NDI_176_pulito_H.fid

Pulse Sequence: s2pul

NDI_176_pulito_C

Sample: NDI_176_pulito_C

File: home/rosini/vnmrsys/data/NDI/NDI_176_pulito_C.fid

Pulse Sequence: s2pul

NDI_115_pulito_H

Sample: NDI_115_pulito_H

File: home/rosini/vnmrsys/data/NDI/NDI_115_pulito_H.fid

Pulse Sequence: s2pul

NDI_115_pulito_C

Sample: NDI_115_pulito_C

File: home/rosini/vnmrsys/data/NDI/NDI_115_pulito_C.fid

Pulse Sequence: s2pul

NDI_053_pulito_H

Sample: NDI_053_pulito_H

File: home/rosini/vnmrsys/data/NDI/NDI_053_pulito_H.fid

Pulse Sequence: s2pul

NDI_115_pulito_C

Sample: NDI_115_pulito_C

File: home/rosini/vnmrsys/data/NDI/NDI_115_pulito_C.fid

Pulse Sequence: s2pul

HPLC traces

Data File S:\4\DATA\NDI\NDI_16_20_B_008.D
Sample Name: NDI_16_20_B

```
=====
Acq. Operator   : Nicola
Acq. Instrument : LC1100DAD                      Location : Vial 30
Injection Date  : 07/05/2013 17.17.11
                                           Inj Volume : 5 µl

Acq. Method     : S:\4\METHODS\NDI\NDI_016_B.M
Last changed    : 07/05/2013 17.13.16 by Nicola
                  (modified after loading)
Analysis Method : C:\HPCHEM\4\METHODS\EF.M
Last changed    : 04/06/2014 11.14.14 by Nicola
                  (modified after loading)
Sample Info     : AD-H HEX/IPA 90/10 0.5 mL/min
=====
```

Area Percent Report

```
=====
Sorted By      : Signal
Multiplier     : 1.0000
Dilution       : 1.0000
Use Multiplier & Dilution Factor with ISTDs
=====
```

Signal 1: DAD1 C, Sig=214,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.366	VB	0.2835	7965.48535	431.14447	43.8422
2	18.798	VB	0.3543	1.02031e4	440.33344	56.1578

Totals : 1.81685e4 871.47791

Data File S:\4\DATA\NDI\NDI_027_B_00000.D
Sample Name: NDI_027_B

```
Acq. Operator   : Nicola
Acq. Instrument : LC1100DAD                      Location : Vial 27
Injection Date  : 28/05/2013 15.48.19
                                                    Inj Volume : 5 µl
Acq. Method     : S:\4\METHODS\NDI\NDI_016_B.M
Last changed    : 23/05/2013 14.46.33 by Nicola
Analysis Method : C:\HPCHEM\4\METHODS\EF.M
Last changed    : 04/06/2014 11.14.14 by Nicola
                  (modified after loading)
Sample Info     : NDI_027_B 0.5 mL/min, 90/10 n-hex/iPA
```

Area Percent Report

```
Sorted By      :      Signal
Multiplier    :      1.0000
Dilution      :      1.0000
Use Multiplier & Dilution Factor with ISTDs
```

Signal 1: DAD1 C, Sig=214,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.100	BB	0.2454	7030.73340	437.68173	100.0000

Totals : 7030.73340 437.68173

*** End of Report ***

Data File S:\4\DATA\NDI\NDI_127_126B_00.D
Sample Name: NDI_127_126B

```
=====
Acq. Operator   : Nicola
Acq. Instrument : LC1100DAD                      Location : Vial 35
Injection Date  : 19/03/2014 14.02.28
                                           Inj Volume : 10 µl

Acq. Method     : C:\HPCHEM\4\METHODS\NDI_095.M
Last changed    : 19/03/2014 13.44.21 by Nicola
                  (modified after loading)
Analysis Method : C:\HPCHEM\4\METHODS\EF.M
Last changed    : 04/06/2014 13.46.41 by Nicola
                  (modified after loading)
Sample Info     : NDI_127_126B; AD-H; Hex/IPA 90/10; 0.5 mL/min
=====
```

```
=====
                          Area Percent Report
=====
```

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	17.308	BB	0.3241	1.19662e4	567.25916	41.0962
2	25.845	BB	0.4928	1.71513e4	536.73389	58.9038

Totals : 2.91175e4 1103.99304

```
=====
*** End of Report ***
=====
```

Data File S:\4\DATA\NDI\NDI_127_000000.D
Sample Name: NDI_127

```
=====
Acq. Operator   : Nicola
Acq. Instrument : LC1100DAD                      Location : Vial 27
Injection Date  : 19/03/2014 15.08.59
                                           Inj Volume : 10 µl

Acq. Method     : C:\HPCHEM\4\METHODS\NDI_095.M
Last changed    : 19/03/2014 13.44.21 by Nicola
                  (modified after loading)
Analysis Method  : C:\HPCHEM\4\METHODS\EF.M
Last changed    : 04/06/2014 13.46.41 by Nicola
                  (modified after loading)
Sample Info     : NDI_127; AD-H; Hex/IPA 90/10; 0.5 mL/min
=====
```

```
=====
                          Area Percent Report
=====
```

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	17.305	MM	0.3587	2.49844e4	1160.71423	99.5228
2	25.821	MM	0.3921	119.80811	5.09196	0.4772

Totals : 2.51042e4 1165.80620

```
=====
*** End of Report ***
=====
```

Data File S:\4\DATA\NDI\NDI_126B_000000.D
Sample Name: NDI_126B

```
=====
Acq. Operator   : Nicola
Acq. Instrument : LC1100DAD                      Location : Vial 36
Injection Date  : 19/03/2014 14.36.03
                                           Inj Volume : 10 µl

Acq. Method     : C:\HPCHEM\4\METHODS\NDI_095.M
Last changed    : 19/03/2014 13.44.21 by Nicola
                  (modified after loading)
Analysis Method : C:\HPCHEM\4\METHODS\EF.M
Last changed    : 04/06/2014 13.46.41 by Nicola
                  (modified after loading)
Sample Info     : NDI_126B; AD-H; Hex/IPA 90/10; 0.5 mL/min
=====
```

```
=====
Area Percent Report
=====
```

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	17.444	BB	0.3238	656.54803	31.16051	1.8319
2	26.280	BB	0.5260	3.51840e4	1011.14923	98.1681

Totals : 3.58406e4 1042.30974

```
=====
*** End of Report ***
=====
```

Data File S:\4\DATA\NDI\NDI_35_36_RACB0.D
Sample Name: NDI_35_36_RACB

```
=====
Acq. Operator   : Nicola
Acq. Instrument : LC1100DAD                      Location : Vial 37
Injection Date  : 11/06/2013 16.59.54
                                           Inj Volume : 5 µl

Acq. Method     : S:\4\METHODS\NDI\NDI_016_B.M
Last changed    : 10/06/2013 12.58.45 by Nicola
Analysis Method : C:\HPCHEM\4\METHODS\EF.M
Last changed    : 04/06/2014 11.14.14 by Nicola
                  (modified after loading)
Sample Info     : NDI_35_36_RACB; 0,5 mL/min; 90/10 hexane/IPA
=====
```

=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 C, Sig=214,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.732	BB	0.2636	2718.82056	158.94138	52.4327
2	19.670	BB	0.3328	2466.52808	113.81756	47.5673

Totals : 5185.34863 272.75893

=====
*** End of Report ***

Data File S:\4\DATA\NDI\NDI_035_B_00000.D
Sample Name: NDI_035_B

```
=====
Acq. Operator   : Nicola
Acq. Instrument : LC1100DAD                      Location : Vial 35
Injection Date  : 11/06/2013 18.06.13
                                           Inj Volume : 5 µl

Acq. Method     : S:\4\METHODS\NDI\NDI_016_B.M
Last changed    : 10/06/2013 12.58.45 by Nicola
Analysis Method : C:\HPCHEM\4\METHODS\EF.M
Last changed    : 04/06/2014 11.14.14 by Nicola
                  (modified after loading)
Sample Info     : NDI_035_B; 0,5 mL/min; 90/10 hexane/IPA
=====
```

=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 C, Sig=214,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	17.785	BB	0.2947	3542.95947	183.97159	100.0000

Totals : 3542.95947 183.97159

=====
*** End of Report ***

Data File S:\4\DATA\NDI\NDI_036_B_00000.D
Sample Name: NDI_036_B

```
=====
Acq. Operator   : Nicola
Acq. Instrument : LC1100DAD                      Location : Vial 36
Injection Date  : 11/06/2013 17.34.33
                                           Inj Volume : 5 µl

Acq. Method     : S:\4\METHODS\NDI\NDI_016_B.M
Last changed    : 10/06/2013 12.58.45 by Nicola
Analysis Method : C:\HPCHEM\4\METHODS\EF.M
Last changed    : 04/06/2014 11.14.14 by Nicola
                  (modified after loading)
Sample Info     : NDI_036_B; 0,5 mL/min; 90/10 hexane/IPA
=====
```

=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 C, Sig=214,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.872	BB	0.2775	86.76247	4.83146	2.7256
2	21.140	BB	0.3576	3096.46191	133.02666	97.2744

Totals : 3183.22439 137.85811

=====
*** End of Report ***

Data File S:\4\DATA\NDI\NDI_29_30_RACB0.D
Sample Name: NDI_29_30_racB

```
=====
Acq. Operator   : Nicola
Acq. Instrument : LC1100DAD                      Location : Vial 31
Injection Date  : 04/06/2013 17.35.51
                                           Inj Volume : 5 µl
Acq. Method     : S:\4\METHODS\NDI\NDI_016_B.M
Last changed    : 28/05/2013 16.46.25 by Nicola
Analysis Method : C:\HPCHEM\4\METHODS\EF.M
Last changed    : 04/06/2014 11.14.14 by Nicola
                  (modified after loading)
Sample Info     : NDI_29_30_racB; 0.5 mL/min; 9/1 hexane/etilacetate AD-H
=====
```

=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 C, Sig=214,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	18.240	BB	0.3203	4103.35889	197.58344	67.3426
2	25.008	BB	0.4563	1989.90417	67.02982	32.6574

Totals : 6093.26306 264.61325

=====
*** End of Report ***

Data File S:\4\DATA\NDI\NDI_29_B_000000.D
Sample Name: NDI_29_B

```
=====
Acq. Operator   : Nicola
Acq. Instrument : LC1100DAD                      Location : Vial 29
Injection Date  : 04/06/2013 18.09.50
                                           Inj Volume : 5 µl

Acq. Method     : S:\4\METHODS\NDI\NDI_016_B.M
Last changed    : 28/05/2013 16.46.25 by Nicola
Analysis Method : C:\HPCHEM\4\METHODS\EF.M
Last changed    : 04/06/2014 11.14.14 by Nicola
                  (modified after loading)
Sample Info     : NDI_29_B; 0.5 mL/min; 9/1 hexane/etilacetate AD-H
=====
```

=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 C, Sig=214,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	19.903	MM	0.3769	5107.66748	225.87054	100.0000

Totals : 5107.66748 225.87054

=====
*** End of Report ***

Data File S:\4\DATA\NDI\NDI_30_B_000000.D
Sample Name: NDI_30_B

```
=====
Acq. Operator   : Nicola
Acq. Instrument : LC1100DAD                      Location : Vial 30
Injection Date  : 04/06/2013 18.43.46
                                           Inj Volume : 5 µl

Acq. Method     : S:\4\METHODS\NDI\NDI_016_B.M
Last changed    : 28/05/2013 16.46.25 by Nicola
Analysis Method : C:\HPCHEM\4\METHODS\EF.M
Last changed    : 04/06/2014 11.14.14 by Nicola
                  (modified after loading)
Sample Info     : NDI_30_B; 0.5 mL/min; 9/1 hexane/etilacetate AD-H
=====
```

```
=====
                        Area Percent Report
=====
```

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 C, Sig=214,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	24.865	BB	0.4541	3048.91870	103.98058	100.0000

Totals : 3048.91870 103.98058

```
=====
*** End of Report ***
=====
```

Data File S:\4\DATA\NDI\NDI_31_32_RACB1.D
Sample Name: NDI_31_32_racB

```
=====
Acq. Operator   : Nicola
Acq. Instrument : LC1100DAD                      Location : Vial 33
Injection Date  : 10/06/2013 10.06.52
                                           Inj Volume : 5 µl

Acq. Method     : S:\4\METHODS\NDI\NDI_016_B.M
Last changed    : 07/06/2013 18.01.42 by Nicola
Analysis Method : C:\HPCHEM\4\METHODS\EF.M
Last changed    : 04/06/2014 11.14.14 by Nicola
                  (modified after loading)
Sample Info     : NDI_31_32_racB; 0,5 mL/min; 90/10 hexane/IPA
=====
```

=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 C, Sig=214,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	20.899	BB	0.3532	3649.66040	158.18286	78.9416
2	27.255	BB	0.4640	973.58099	32.44851	21.0584

Totals : 4623.24139 190.63137

=====
*** End of Report ***

Data File S:\4\DATA\NDI\NDI_031_B_00000.D
Sample Name: NDI_031_B

```
=====
Acq. Operator   : Nicola
Acq. Instrument : LC1100DAD                      Location : Vial 31
Injection Date  : 10/06/2013 11.56.46
                                           Inj Volume : 5 µl
Acq. Method     : S:\4\METHODS\NDI\NDI_016_B.M
Last changed    : 07/06/2013 18.01.42 by Nicola
Analysis Method : C:\HPCHEM\4\METHODS\EF.M
Last changed    : 04/06/2014 11.14.14 by Nicola
                  (modified after loading)
Sample Info     : NDI_031_B; 0,5 mL/min; 90/10 hexane/IPA
=====
```

=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 C, Sig=214,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	21.388	BB	0.3619	4942.21533	210.47620	100.0000

Totals : 4942.21533 210.47620

=====
*** End of Report ***

Data File S:\4\DATA\NDI\NDI_032_B_00000.D
Sample Name: NDI_032_B

```
=====
Acq. Operator   : Nicola
Acq. Instrument : LC1100DAD                      Location : Vial 32
Injection Date  : 10/06/2013 11.08.04
                                           Inj Volume : 5 µl

Acq. Method     : S:\4\METHODS\NDI\NDI_016_B.M
Last changed    : 07/06/2013 18.01.42 by Nicola
Analysis Method : C:\HPCHEM\4\METHODS\EF.M
Last changed    : 04/06/2014 11.14.14 by Nicola
                  (modified after loading)
Sample Info     : NDI_032_B_; 0,5 mL/min; 90/10 hexane/IPA
=====
```

=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 C, Sig=214,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	25.266	BB	0.4375	1280.97021	45.34925	100.0000

Totals : 1280.97021 45.34925

=====
*** End of Report ***

Data File S:\4\DATA\NDI\NDI_41_42_BRAC0.D
Sample Name: NDI_41_42_Brac

```
=====
Acq. Operator   : Nicola
Acq. Instrument : LC1100DAD                      Location : Vial 43
Injection Date  : 13/06/2013 11.50.41
                                           Inj Volume : 5 µl
Acq. Method     : S:\4\METHODS\NDI\NDI_016_B.M
Last changed    : 12/06/2013 18.41.08 by Nicola
Analysis Method : C:\HPCHEM\4\METHODS\EF.M
Last changed    : 04/06/2014 11.14.14 by Nicola
                  (modified after loading)
Sample Info     : NDI_41_42_Brac; 0,5 mL/min; 90/10 hexane/IPA
=====
```

=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 C, Sig=214,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.264	BB	0.2378	2411.32983	154.75241	34.1112
2	18.343	BB	0.3159	4657.70557	226.52980	65.8888

Totals : 7069.03540 381.28221

=====
*** End of Report ***

Data File S:\4\DATA\NDI\NDI_041_B_00000.D
Sample Name: NDI_041_B

```
=====
Acq. Operator   : Nicola
Acq. Instrument : LC1100DAD                      Location : Vial 41
Injection Date  : 13/06/2013 12.55.58
                                           Inj Volume : 5 µl

Acq. Method     : S:\4\METHODS\NDI\NDI_016_B.M
Last changed    : 12/06/2013 18.41.08 by Nicola
Analysis Method : C:\HPCHEM\4\METHODS\EF.M
Last changed    : 04/06/2014 12.06.17 by Nicola
                  (modified after loading)
Sample Info     : NDI_041_B; 0,5 mL/min; 90/10 hexane/IPA
=====
```

=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 C, Sig=214,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.931	BB	0.2501	3448.53125	211.60091	100.0000

Totals : 3448.53125 211.60091

=====
*** End of Report ***

Data File S:\4\DATA\NDI\NDI_042_B_00000.D
Sample Name: NDI_042_B

```
Acq. Operator   : Nicola
Acq. Instrument : LC1100DAD                      Location : Vial 42
Injection Date  : 13/06/2013 12.17.44
                                           Inj Volume : 5 µl
Acq. Method     : S:\4\METHODS\NDI\NDI_016_B.M
Last changed    : 12/06/2013 18.41.08 by Nicola
Analysis Method : C:\HPCHEM\4\METHODS\EF.M
Last changed    : 04/06/2014 11.14.14 by Nicola
                  (modified after loading)
Sample Info     : NDI_042_B; 0,5 mL/min; 90/10 hexane/IPA
```

Area Percent Report

```
Sorted By      :      Signal
Multiplier    :      1.0000
Dilution      :      1.0000
Use Multiplier & Dilution Factor with ISTDs
```

Signal 1: DAD1 C, Sig=214,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.277	BB	0.2330	155.46033	10.13247	3.0244
2	18.337	BB	0.3153	4984.76221	243.01440	96.9756

Totals : 5140.22253 253.14687

*** End of Report ***

Data File S:\4\DATA\NDI\NDI_39_40_BRAC0.D
Sample Name: NDI_39_40_Brac

```
=====
Acq. Operator   : Nicola
Acq. Instrument : LC1100DAD                      Location : Vial 41
Injection Date  : 12/06/2013 16.47.11
                                           Inj Volume : 5 µl

Acq. Method     : S:\4\METHODS\NDI\NDI_016_B.M
Last changed    : 11/06/2013 18.36.40 by Nicola
Analysis Method : C:\HPCHEM\4\METHODS\EF.M
Last changed    : 04/06/2014 11.14.14 by Nicola
                  (modified after loading)
Sample Info     : NDI_39_40_Brac; 0,5 mL/min; 90/10 hexane/IPA
=====
```

=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 C, Sig=214,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	18.908	BB	0.3143	3983.34766	194.99290	73.1800
2	25.191	BB	0.4246	1459.86768	53.11676	26.8200

Totals : 5443.21533 248.10966

=====
*** End of Report ***

Data File S:\4\DATA\NDI\NDI_039_B_00000.D
Sample Name: NDI_039_B

```
=====
Acq. Operator   : Nicola
Acq. Instrument : LC1100DAD                      Location : Vial 39
Injection Date  : 12/06/2013 18.05.36
                                           Inj Volume : 5 µl

Acq. Method     : S:\4\METHODS\NDI\NDI_016_B.M
Last changed    : 11/06/2013 18.36.40 by Nicola
Analysis Method : C:\HPCHEM\4\METHODS\EF.M
Last changed    : 04/06/2014 11.14.14 by Nicola
                  (modified after loading)
Sample Info     : NDI_039_B; 0,5 mL/min; 90/10 hexane/IPA
=====
```

=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 C, Sig=214,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.196	BB	0.2771	5243.69434	292.55521	100.0000

Totals : 5243.69434 292.55521

=====
*** End of Report ***

Data File S:\4\DATA\NDI\NDI_040_B_00000.D
Sample Name: NDI_040_B

```
=====
Acq. Operator   : Nicola
Acq. Instrument : LC1100DAD                      Location : Vial 40
Injection Date  : 12/06/2013 17.31.30
                                           Inj Volume : 5 µl

Acq. Method     : S:\4\METHODS\NDI\NDI_016_B.M
Last changed    : 11/06/2013 18.36.40 by Nicola
Analysis Method : C:\HPCHEM\4\METHODS\EF.M
Last changed    : 04/06/2014 11.14.14 by Nicola
                  (modified after loading)
Sample Info     : NDI_040_B; 0,5 mL/min; 90/10 hexane/IPA
=====
```

=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 C, Sig=214,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	24.261	BB	0.4081	1586.53650	60.07185	100.0000

Totals : 1586.53650 60.07185

=====
*** End of Report ***

Data File S:\4\DATA\NDI\NDI_37_38_BRAC0.D
Sample Name: NDI_37_38_BRAC

```
=====
Acq. Operator   : Nicola
Acq. Instrument : LC1100DAD                      Location : Vial 39
Injection Date  : 12/06/2013 14.01.49
                                           Inj Volume : 5 µl

Acq. Method     : S:\4\METHODS\NDI\NDI_016_B.M
Last changed    : 11/06/2013 18.36.40 by Nicola
Analysis Method : C:\HPCHEM\4\METHODS\EF.M
Last changed    : 04/06/2014 11.14.14 by Nicola
                  (modified after loading)
Sample Info     : NDI_37_38_Brac; 0,5 mL/min; 90/10 hexane/IPA
=====
```

=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 C, Sig=214,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	17.278	BB	0.2978	2372.02417	122.57104	47.9563
2	23.154	BB	0.4125	2574.19287	96.10656	52.0437

Totals : 4946.21704 218.67760

=====
*** End of Report ***

Data File S:\4\DATA\NDI\NDI_037_B_00000.D
Sample Name: NDI_037_B

```
=====
Acq. Operator   : Nicola
Acq. Instrument : LC1100DAD                      Location : Vial 37
Injection Date  : 12/06/2013 15.44.38
                                           Inj Volume : 5 µl

Acq. Method     : S:\4\METHODS\NDI\NDI_016_B.M
Last changed    : 11/06/2013 18.36.40 by Nicola
Analysis Method : C:\HPCHEM\4\METHODS\EF.M
Last changed    : 04/06/2014 11.14.14 by Nicola
                  (modified after loading)
Sample Info     : NDI_037_B; 0,5 mL/min; 90/10 hexane/IPA
=====
```

=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 C, Sig=214,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	19.377	BB	0.3264	2241.10693	105.25674	100.0000

Totals : 2241.10693 105.25674

=====
*** End of Report ***

Data File S:\4\DATA\NDI\NDI_038_B_00000.D
Sample Name: NDI_038_B

```
Acq. Operator   : Nicola
Acq. Instrument : LC1100DAD                      Location : Vial 38
Injection Date  : 12/06/2013 14.46.36
                                           Inj Volume : 5 µl
Acq. Method     : S:\4\METHODS\NDI\NDI_016_B.M
Last changed    : 11/06/2013 18.36.40 by Nicola
Analysis Method : C:\HPCHEM\4\METHODS\EF.M
Last changed    : 04/06/2014 11.14.14 by Nicola
                  (modified after loading)
Sample Info     : NDI_038_B; 0,5 mL/min; 90/10 hexane/IPA
```

Area Percent Report

```
Sorted By      :      Signal
Multiplier    :      1.0000
Dilution      :      1.0000
Use Multiplier & Dilution Factor with ISTDs
```

Signal 1: DAD1 C, Sig=214,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	26.281	BB	0.4577	2802.59180	94.03549	100.0000

Totals :	2802.59180	94.03549
----------	------------	----------

*** End of Report ***

Data File S:\4\DATA\NDI\NDI_180_181_002.D
Sample Name: NDI_180_181

```
Acq. Operator   : Nicola
Acq. Instrument : LC1100DAD                      Location : Vial 82
Injection Date  : 02/07/2014 13.03.49
                                           Inj Volume : 10 µl
Acq. Method     : C:\HPCHEM\4\METHODS\NDI_095.M
Last changed    : 02/07/2014 12.31.48 by Nicola
                  (modified after loading)
Analysis Method : C:\HPCHEM\4\METHODS\NDI_095.M
Last changed    : 01/07/2014 18.30.42 by Nicola
Sample Info     : NDI_180_181; AD-H; Hex/IPA 95/5; 0.5 mL/min;
```

Area Percent Report

```
Sorted By      :      Signal
Multiplier    :      1.0000
Dilution      :      1.0000
Use Multiplier & Dilution Factor with ISTDs
```

Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.089	VV	0.2797	2.87875e4	1601.60181	70.0883
2	15.913	BV	0.3027	1.22857e4	621.39386	29.9117

Totals : 4.10732e4 2222.99567

*** End of Report ***

Data File S:\4\DATA\NDI\NDI_180_000000.D
Sample Name: NDI_180

```
=====
Acq. Operator   : Nicola
Acq. Instrument : LC1100DAD                      Location : Vial 80
Injection Date  : 02/07/2014 14.29.17
                                           Inj Volume : 10 µl

Acq. Method     : C:\HPCHEM\4\METHODS\NDI_095.M
Last changed    : 02/07/2014 12.31.48 by Nicola
                  (modified after loading)
Analysis Method : C:\HPCHEM\4\METHODS\NDI_095.M
Last changed    : 01/07/2014 18.30.42 by Nicola
Sample Info     : NDI_180; AD-H; Hex/IPA 95/5; 0.5 mL/min;
=====
```

Area Percent Report

```
=====
Sorted By      : Signal
Multiplier     : 1.0000
Dilution       : 1.0000
Use Multiplier & Dilution Factor with ISTDs
=====
```

Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.060	MM	0.3672	4.75137e4	2156.53247	99.5639
2	15.904	MM	0.3092	208.12544	11.21758	0.4361

Totals : 4.77218e4 2167.75005

*** End of Report ***

Data File S:\4\DATA\NDI\NDI_181_000000.D
Sample Name: NDI_181

```
=====
Acq. Operator   : Nicola
Acq. Instrument : LC1100DAD                      Location : Vial 81
Injection Date  : 02/07/2014 14.51.36
                                           Inj Volume : 10 µl

Acq. Method     : C:\HPCHEM\4\METHODS\NDI_095.M
Last changed    : 02/07/2014 12.31.48 by Nicola
                  (modified after loading)
Analysis Method : C:\HPCHEM\4\METHODS\NDI_095.M
Last changed    : 01/07/2014 18.30.42 by Nicola
Sample Info     : NDI_181; AD-H; Hex/IPA 95/5; 0.5 mL/min;
=====
```

=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.101	VV	0.2497	300.00677	18.45415	1.1565
2	15.892	VB	0.2943	2.56405e4	1333.46936	98.8435

Totals : 2.59405e4 1351.92351

=====
*** End of Report ***

Data File S:\4\DATA\NDI\NDI_136_138B_01.D
Sample Name: NDI_136_138B

```
=====
Acq. Operator   : NDI
Acq. Instrument : LC1100DAD                      Location : Vial 34
Injection Date  : 09/04/2014 13.59.24
                                           Inj Volume : 10 µl

Acq. Method     : C:\HPCHEM\4\METHODS\NDI_095.M
Last changed    : 09/04/2014 13.58.09 by NDI
                  (modified after loading)
Analysis Method : C:\HPCHEM\4\METHODS\EF.M
Last changed    : 04/06/2014 13.46.41 by Nicola
                  (modified after loading)
Sample Info     : NDI_136_138B; AD-H; Hex/IPA 95/5; 0.5 mL/min
=====
```

```
=====
                          Area Percent Report
=====
```

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	19.230	BB	0.3477	7637.89014	337.94260	42.3856
2	24.042	BB	0.5281	1.03821e4	289.73517	57.6144

Totals : 1.80200e4 627.67776

```
=====
*** End of Report ***
=====
```

Data File S:\4\DATA\NDI\NDI_136_000000.D
Sample Name: NDI_136

```
=====
Acq. Operator   : NDI
Acq. Instrument : LC1100DAD                      Location : Vial 36
Injection Date  : 09/04/2014 15.33.29
                                           Inj Volume : 10 µl

Acq. Method     : C:\HPCHEM\4\METHODS\NDI_095.M
Last changed    : 09/04/2014 13.58.09 by NDI
                  (modified after loading)
Analysis Method : C:\HPCHEM\4\METHODS\EF.M
Last changed    : 04/06/2014 13.46.41 by Nicola
                  (modified after loading)
Sample Info     : NDI_136; AD-H; Hex/IPA 95/5; 0.5 mL/min
=====
```

```
=====
                          Area Percent Report
=====
```

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	19.108	BB	0.3470	1.55208e4	688.50903	99.6230
2	24.480	BB	0.3825	58.73910	2.23553	0.3770

Totals : 1.55796e4 690.74456

```
=====
*** End of Report ***
=====
```

Data File S:\4\DATA\NDI\NDI_138B_000000.D
Sample Name: NDI_138B

```
=====
Acq. Operator   : NDI
Acq. Instrument : LC1100DAD                      Location : Vial 46
Injection Date  : 09/04/2014 16.59.19
                                           Inj Volume : 10 µl

Acq. Method     : C:\HPCHEM\4\METHODS\NDI_095.M
Last changed    : 09/04/2014 13.58.09 by NDI
                  (modified after loading)
Analysis Method : C:\HPCHEM\4\METHODS\EF.M
Last changed    : 04/06/2014 13.46.41 by Nicola
                  (modified after loading)
Sample Info     : NDI_138B; AD-H; Hex/IPA 95/5; 0.5 mL/min
=====
```

```
=====
                          Area Percent Report
=====
```

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	23.830	BB	0.5119	1.99606e4	573.73120	100.0000

Totals : 1.99606e4 573.73120

```
=====
*** End of Report ***
=====
```

Data File S:\4\DATA\NDI\NDI139_40_41_13.D
Sample Name: NDI_139_40_41

```
Acq. Operator   : Nicola
Acq. Instrument : LC1100DAD                      Location : Vial 38
Injection Date  : 04/06/2014 15.45.21
                                                    Inj Volume : 10 µl

Acq. Method     : C:\HPCHEM\4\METHODS\EF.M
Last changed    : 04/06/2014 15.39.39 by Nicola
                  (modified after loading)
Analysis Method : C:\HPCHEM\4\METHODS\EF.M
Last changed    : 05/06/2014 11.55.37 by Nicola
                  (modified after loading)
Sample Info     : NDI_139_40_41; cellulose; 90/10 Hex/IPA; 0.5 mL/min
```

Area Percent Report

```
Sorted By      :      Signal
Multiplier    :      1.0000
Dilution      :      1.0000
Use Multiplier & Dilution Factor with ISTDs
```

Signal 1: DAD1 C, Sig=214,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	36.773	MF	1.3946	4964.15625	59.32471	27.6164
2	50.071	FM	4.0141	1.30112e4	54.02368	72.3836

Totals :	1.79754e4	113.34839
----------	-----------	-----------

*** End of Report ***

Data File S:\4\DATA\NDI\NDI_139_000003.D
Sample Name: NDI_139

```
=====
Acq. Operator   : Nicola
Acq. Instrument : LC1100DAD                      Location : Vial 39
Injection Date  : 04/06/2014 16.48.53
                                           Inj Volume : 10 µl

Acq. Method     : C:\HPCHEM\4\METHODS\EF.M
Last changed    : 04/06/2014 15.39.39 by Nicola
                  (modified after loading)
Analysis Method : C:\HPCHEM\4\METHODS\EF.M
Last changed    : 05/06/2014 11.55.37 by Nicola
                  (modified after loading)
Sample Info     : NDI_139; cellulose; 90/10 Hex/IPA; 0.5 mL/min
=====
```

```
=====
Area Percent Report
=====
```

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 C, Sig=214,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	49.533	BB	2.9049	4.45627e4	204.45473	100.0000

Totals : 4.45627e4 204.45473

```
=====
*** End of Report ***
=====
```

Data File S:\4\DATA\NDI\NDI_144_146B_01.D
Sample Name: NDI_144_146B

```
=====
Acq. Operator   : Nicola
Acq. Instrument : LC1100DAD                      Location : Vial 42
Injection Date  : 23/04/2014 9.12.35
                                           Inj Volume : 10 µl

Acq. Method     : C:\HPCHEM\4\METHODS\NDI_095.M
Last changed    : 23/04/2014 9.09.25 by Nicola
                  (modified after loading)
Analysis Method : C:\HPCHEM\4\METHODS\EF.M
Last changed    : 04/06/2014 13.46.41 by Nicola
                  (modified after loading)
Sample Info     : NDI_144_146B; AD-H; Hex/IPA 95/5; 0.5 mL/min
=====
```

=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	38.302	BB	0.7244	6276.30029	133.04004	34.8241
2	43.207	BV	0.8328	1.17466e4	217.24966	65.1759

Totals : 1.80229e4 350.28970

=====
*** End of Report ***

Data File S:\4\DATA\NDI\NDI_144_000000.D
Sample Name: NDI_144

```
=====
Acq. Operator   : Nicola
Acq. Instrument : LC1100DAD                      Location : Vial 44
Injection Date  : 23/04/2014 10.10.53
                                           Inj Volume : 10 µl

Acq. Method     : C:\HPCHEM\4\METHODS\NDI_095.M
Last changed    : 23/04/2014 9.09.25 by Nicola
                  (modified after loading)
Analysis Method : C:\HPCHEM\4\METHODS\EF.M
Last changed    : 04/06/2014 13.46.41 by Nicola
                  (modified after loading)
Sample Info     : NDI_144; AD-H; Hex/IPA 95/5; 0.5 mL/min
=====
```

=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	38.834	MM	0.8555	499.54559	9.73195	2.1231
2	43.357	MM	0.9387	2.30296e4	408.88947	97.8769

Totals : 2.35291e4 418.62141

=====
*** End of Report ***

Data File S:\4\DATA\NDI\NDI_146B_VERO_0.D
Sample Name: NDI_146B_vero

```
=====
Acq. Operator   : Nicola
Acq. Instrument : LC1100DAD                      Location : Vial 54
Injection Date  : 23/04/2014 11.22.40
                                           Inj Volume : 10 µl

Acq. Method     : C:\HPCHEM\4\METHODS\NDI_095.M
Last changed    : 23/04/2014 9.09.25 by Nicola
                  (modified after loading)
Analysis Method : C:\HPCHEM\4\METHODS\EF.M
Last changed    : 04/06/2014 13.46.41 by Nicola
                  (modified after loading)
Sample Info     : NDI_146B_vero; AD-H; Hex/IPA 95/5; 0.5 mL/min
=====
```

=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	38.520	BB	0.7180	1.12615e4	243.30629	100.0000

Totals : 1.12615e4 243.30629

=====
*** End of Report ***

Data File S:\4\DATA\NDI\NDI_17_20_RAC08.D
Sample Name: NDI_17_20_rac

```
=====
Acq. Operator   : Nicola
Acq. Instrument : LC1100DAD                      Location : Vial 29
Injection Date  : 30/05/2013 11.14.18             Inj Volume : 5 µl
Acq. Method     : S:\4\METHODS\NDI\NDI_016_A.M
Last changed    : 23/05/2013 19.00.15 by Nicola
Analysis Method : C:\HPCHEM\4\METHODS\EF.M
Last changed    : 04/06/2014 11.14.14 by Nicola
                  (modified after loading)
Sample Info     : NDI_17_20_rac Hex/IPA=90-10 0.75mL/min
=====
```

=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 C, Sig=214,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	20.180	BB	0.7279	5812.92529	124.22849	48.0012
2	25.354	BB	0.9424	6297.04395	102.82868	51.9988

Totals : 1.21100e4 227.05717

=====
*** End of Report ***

Data File S:\4\DATA\NDI\NDI_028_A_00000.D
Sample Name: NDI_028_A

```
=====
Acq. Operator   : Nicola
Acq. Instrument : LC1100DAD                      Location : Vial 28
Injection Date  : 30/05/2013 11.47.40
                                           Inj Volume : 5 µl

Acq. Method     : S:\4\METHODS\NDI\NDI_016_A.M
Last changed    : 23/05/2013 19.00.15 by Nicola
Analysis Method : C:\HPCHEM\4\METHODS\EF.M
Last changed    : 04/06/2014 11.14.14 by Nicola
                  (modified after loading)
Sample Info     : NDI_028_A Hex/IPA=90-10 0.75mL/min
=====
```

=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 C, Sig=214,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	20.793	BB	0.7246	2465.47852	52.81875	100.0000

Totals : 2465.47852 52.81875

=====
*** End of Report ***

Data File S:\4\DATA\NDI\NDI_20_A_000010.D
Sample Name: NDI_20_A

```
=====
Acq. Operator   : Nicola
Acq. Instrument : LC1100DAD                      Location : Vial 21
Injection Date  : 08/05/2013 18.46.19
                                           Inj Volume : 5 µl

Acq. Method     : S:\4\METHODS\NDI\NDI_016_A.M
Last changed    : 08/05/2013 18.44.15 by Nicola
                  (modified after loading)
Analysis Method : C:\HPCHEM\4\METHODS\EF.M
Last changed    : 04/06/2014 11.14.14 by Nicola
                  (modified after loading)
Sample Info     : OD-H - HEX/IPA 90/10 - 0.75 mL/min
=====
```

=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 C, Sig=214,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	19.653	BB	0.5728	169.68698	4.11737	0.9589
2	24.989	VB	0.9287	1.75262e4	292.62799	99.0411

Totals : 1.76959e4 296.74536

Data File S:\4\DATA\NDI\NDI_125_126A_00.D
Sample Name: NDI_125_126A

```
=====
Acq. Operator   : Nicola
Acq. Instrument : LC1100DAD                      Location : Vial 34
Injection Date  : 19/03/2014 10.19.08
                                           Inj Volume : 10 µl

Acq. Method     : C:\HPCHEM\4\METHODS\NDI_095.M
Last changed    : 19/03/2014 9.27.26 by Nicola
                  (modified after loading)
Analysis Method : C:\HPCHEM\4\METHODS\EF.M
Last changed    : 04/06/2014 13.46.41 by Nicola
                  (modified after loading)
Sample Info     : NDI_125_126A; AD-H; Hex/IPA 95/5; 1 mL/min
=====
```

=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.919	BV	0.3401	7619.93262	336.64050	49.6547
2	15.924	VB	0.3637	7725.90381	324.52472	50.3453

Totals : 1.53458e4 661.16522

=====
*** End of Report ***

Data File S:\4\DATA\NDI\NDI_125_000000.D
Sample Name: NDI_125

```
=====
Acq. Operator   : Nicola
Acq. Instrument : LC1100DAD                      Location : Vial 25
Injection Date  : 19/03/2014 10.47.01
                                           Inj Volume : 10 µl

Acq. Method     : C:\HPCHEM\4\METHODS\NDI_095.M
Last changed    : 19/03/2014 9.27.26 by Nicola
                  (modified after loading)
Analysis Method : C:\HPCHEM\4\METHODS\EF.M
Last changed    : 04/06/2014 13.46.41 by Nicola
                  (modified after loading)
Sample Info     : NDI_125; AD-H; Hex/IPA 95/5; 1 mL/min
=====
```

=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.823	BB	0.3372	1.51280e4	675.77222	100.0000

Totals : 1.51280e4 675.77222

=====
*** End of Report ***

Data File S:\4\DATA\NDI\NDI_126A_000000.D
Sample Name: NDI_126A

```
=====
Acq. Operator   : Nicola
Acq. Instrument : LC1100DAD                      Location : Vial 26
Injection Date  : 19/03/2014 13.03.09
                                           Inj Volume : 10 µl

Acq. Method     : C:\HPCHEM\4\METHODS\NDI_095.M
Last changed    : 19/03/2014 13.01.50 by Nicola
                  (modified after loading)
Analysis Method : C:\HPCHEM\4\METHODS\EF.M
Last changed    : 04/06/2014 13.46.41 by Nicola
                  (modified after loading)
Sample Info     : NDI_126A; AD-H; Hex/IPA 95/5; 1 mL/min
=====
```

Area Percent Report

```
Sorted By      : Signal
Multiplier     : 1.0000
Dilution       : 1.0000
Use Multiplier & Dilution Factor with ISTDs
```

Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.818	BV	0.3420	222.21092	10.04969	1.4353
2	15.513	VV	0.3511	1.52593e4	666.45892	98.5647

Totals : 1.54815e4 676.50862

*** End of Report ***

Data File S:\4\DATA\NDI\NDI_097_098_006.D
Sample Name: NDI_097_098

```
=====
Acq. Operator   : Nicola
Acq. Instrument : LC1100DAD                      Location : Vial 61
Injection Date  : 05/06/2014 17.05.14
                                           Inj Volume : 10 µl

Acq. Method     : C:\HPCHEM\4\METHODS\EF.M
Last changed    : 05/06/2014 16.40.34 by Nicola
                  (modified after loading)
Analysis Method : C:\HPCHEM\4\METHODS\EF.M
Last changed    : 05/06/2014 11.55.37 by Nicola
                  (modified after loading)
Sample Info     : NDI_097_098; AD-H; 95/5 Hex/IPA; 1 mL/min
=====
```

=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 C, Sig=214,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.445	MM	0.4375	5457.65234	207.92191	52.8912
2	17.011	MM	0.4069	4860.98730	199.12888	47.1088

Totals : 1.03186e4 407.05078

=====
*** End of Report ***

Data File S:\4\DATA\NDI\NDI_097_000000.D
Sample Name: NDI_097

```
=====
Acq. Operator   : Nicola
Acq. Instrument : LC1100DAD                      Location : Vial 97
Injection Date  : 07/02/2014 15.14.21
                                           Inj Volume : 10 µl

Acq. Method     : C:\HPCHEM\4\METHODS\NDI_095.M
Last changed    : 07/02/2014 13.53.51 by Nicola
                  (modified after loading)
Analysis Method : C:\HPCHEM\4\METHODS\EF.M
Last changed    : 04/06/2014 12.40.17 by Nicola
                  (modified after loading)
Sample Info     : NDI_097; AD-H; 95/5 esano/ipa; 1 mL/min;
=====
```

=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 C, Sig=214,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	17.380	BB	0.4031	2.85537e4	1091.79578	100.0000

Totals : 2.85537e4 1091.79578

=====
*** End of Report ***

Data File S:\4\DATA\NDI\NDI_098_000000.D
Sample Name: NDI_098

```
=====
Acq. Operator   : Nicola
Acq. Instrument : LC1100DAD                      Location : Vial 98
Injection Date  : 07/02/2014 14.38.02
                                           Inj Volume : 10 µl

Acq. Method     : C:\HPCHEM\4\METHODS\NDI_095.M
Last changed    : 07/02/2014 13.53.51 by Nicola
                  (modified after loading)
Analysis Method : C:\HPCHEM\4\METHODS\EF.M
Last changed    : 04/06/2014 12.40.17 by Nicola
                  (modified after loading)
Sample Info     : NDI_098; AD-H; 95/5 esano/ipa; 1 mL/min;
=====
```

=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 C, Sig=214,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.017	MM	0.4336	4097.43311	157.49529	100.0000

Totals : 4097.43311 157.49529

=====
*** End of Report ***

Data File S:\4\DATA\NDI\NDI_099_100_004.D
Sample Name: NDI_099_100

```
=====
Acq. Operator   : Nicola
Acq. Instrument : LC1100DAD                      Location : Vial 62
Injection Date  : 05/06/2014 16.44.50
                                           Inj Volume : 10 µl

Acq. Method     : C:\HPCHEM\4\METHODS\EF.M
Last changed    : 05/06/2014 16.40.34 by Nicola
                  (modified after loading)
Analysis Method : C:\HPCHEM\4\METHODS\EF.M
Last changed    : 05/06/2014 11.55.37 by Nicola
                  (modified after loading)
Sample Info     : NDI_099_100; AD-H; 95/5 Hex/IPA; 1 mL/min
=====
```

=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 C, Sig=214,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.491	VB	0.2575	3173.23193	187.44307	46.7472
2	14.838	BB	0.3267	3614.84155	170.93446	53.2528

Totals : 6788.07349 358.37753

=====
*** End of Report ***

Data File S:\4\DATA\NDI\NDI_099_000000.D
Sample Name: NDI_099

```
=====
Acq. Operator   : Nicola
Acq. Instrument : LC1100DAD                      Location : Vial 99
Injection Date  : 07/02/2014 16.00.19
                                           Inj Volume : 10 µl

Acq. Method     : C:\HPCHEM\4\METHODS\NDI_095.M
Last changed    : 07/02/2014 13.53.51 by Nicola
                  (modified after loading)
Analysis Method : C:\HPCHEM\4\METHODS\EF.M
Last changed    : 04/06/2014 12.40.17 by Nicola
                  (modified after loading)
Sample Info     : NDI_099; AD-H; 95/5 esano/ipa; 1 mL/min;
=====
```

=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 C, Sig=214,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.040	BB	0.3466	2.34394e4	1041.30042	100.0000

Totals : 2.34394e4 1041.30042

=====
*** End of Report ***

Data File S:\4\DATA\NDI\NDI_100_000000.D
Sample Name: NDI_100

```
=====
Acq. Operator   : Nicola
Acq. Instrument : LC1100DAD                      Location : Vial 100
Injection Date  : 07/02/2014 16.38.10
                                           Inj Volume : 10 µl

Acq. Method     : C:\HPCHEM\4\METHODS\NDI_095.M
Last changed    : 07/02/2014 13.53.51 by Nicola
                  (modified after loading)
Analysis Method : C:\HPCHEM\4\METHODS\EF.M
Last changed    : 04/06/2014 12.40.17 by Nicola
                  (modified after loading)
Sample Info     : NDI_100; AD-H; 95/5 esano/ipa; 1 mL/min;
=====
```

=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 C, Sig=214,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.810	VB	0.2942	5453.44580	286.29453	98.3224
2	15.315	MM	0.4463	93.05055	3.47451	1.6776

Totals : 5546.49635 289.76904

=====
*** End of Report ***

Data File S:\4\DATA\NDI\NDI_109_110_002.D
Sample Name: NDI_109_110

```
=====
Acq. Operator   : Nicola
Acq. Instrument : LC1100DAD                      Location : Vial 5
Injection Date  : 27/02/2014 14.43.48
                                           Inj Volume : 10 µl

Acq. Method     : C:\HPCHEM\4\METHODS\NDI_095.M
Last changed    : 27/02/2014 14.42.27 by Nicola
                  (modified after loading)
Analysis Method : C:\HPCHEM\4\METHODS\EF.M
Last changed    : 04/06/2014 13.43.38 by Nicola
                  (modified after loading)
Sample Info     : NDI_109_110; AD-H; 95/5 esano/ipa; 0.5 mL/min;
=====
```

=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	36.337	BV	0.6867	6628.85840	149.68613	38.7373
2	38.154	VB	0.7156	1.04835e4	226.65823	61.2627

Totals : 1.71123e4 376.34436

=====
*** End of Report ***

Data File S:\4\DATA\NDI\NDI_109_000000.D
Sample Name: NDI_109

```
=====
Acq. Operator   : Nicola
Acq. Instrument : LC1100DAD                      Location : Vial 9
Injection Date  : 27/02/2014 15.53.45
                                           Inj Volume : 10 µl

Acq. Method     : C:\HPCHEM\4\METHODS\NDI_095.M
Last changed    : 27/02/2014 14.42.27 by Nicola
                  (modified after loading)
Analysis Method : C:\HPCHEM\4\METHODS\EF.M
Last changed    : 04/06/2014 13.43.38 by Nicola
                  (modified after loading)
Sample Info     : NDI_109; AD-H; 95/5 esano/ipa; 0.5 mL/min;
=====
```

=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	38.126	BB	0.7150	2.11117e4	458.69635	100.0000

Totals : 2.11117e4 458.69635

=====
*** End of Report ***

Data File S:\4\DATA\NDI\NDI_110_000000.D
Sample Name: NDI_110

```
=====
Acq. Operator   : Nicola
Acq. Instrument : LC1100DAD                      Location : Vial 10
Injection Date  : 27/02/2014 16.48.49
                                           Inj Volume : 10 µl

Acq. Method     : C:\HPCHEM\4\METHODS\NDI_095.M
Last changed    : 27/02/2014 14.42.27 by Nicola
                  (modified after loading)
Analysis Method : C:\HPCHEM\4\METHODS\EF.M
Last changed    : 04/06/2014 13.45.46 by Nicola
                  (modified after loading)
Sample Info     : NDI_110; AD-H; 95/5 esano/ipa; 0.5 mL/min;
=====
```

=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	36.227	BB	0.6801	1.31798e4	297.95251	100.0000

Totals : 1.31798e4 297.95251

=====
*** End of Report ***

Data File S:\4\DATA\NDI\NDI_101_102_000.D
Sample Name: NDI_101_102

```
=====
Acq. Operator   : Nicola
Acq. Instrument : LC1100DAD                      Location : Vial 94
Injection Date  : 06/02/2014 18.45.39
                                           Inj Volume : 10 µl

Acq. Method     : C:\HPCHEM\4\METHODS\NDI_095.M
Last changed    : 06/02/2014 14.00.34 by Nicola
                  (modified after loading)
Analysis Method : C:\HPCHEM\4\METHODS\EF.M
Last changed    : 04/06/2014 12.40.17 by Nicola
                  (modified after loading)
Sample Info     : NDI_101_102; AD-H 95/5 esano/ipa; 1 mL/min;
=====
```

=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.602	BB	0.2317	5352.65967	355.35034	45.4260
2	14.437	BB	0.3421	6430.58105	284.09866	54.5740

Totals : 1.17832e4 639.44901

=====
*** End of Report ***

Data File S:\4\DATA\NDI\NDI_101_000000.D
Sample Name: NDI_101

```
=====
Acq. Operator   : Nicola
Acq. Instrument : LC1100DAD                      Location : Vial 1
Injection Date  : 06/02/2014 19.21.06              Inj Volume : 10 µl

Acq. Method     : C:\HPCHEM\4\METHODS\NDI_095.M
Last changed    : 06/02/2014 14.00.34 by Nicola
                  (modified after loading)
Analysis Method : C:\HPCHEM\4\METHODS\EF.M
Last changed    : 04/06/2014 12.40.17 by Nicola
                  (modified after loading)
Sample Info     : NDI_101; AD-H 95/5 esano/ipa; 1 mL/min;
=====
```

=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 C, Sig=214,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.608	VB	0.2869	3.42410e4	1894.23865	100.0000

Totals : 3.42410e4 1894.23865

=====
*** End of Report ***

Data File S:\4\DATA\NDI\NDI_102_000000.D
Sample Name: NDI_102

```
=====
Acq. Operator   : Nicola
Acq. Instrument : LC1100DAD                      Location : Vial 2
Injection Date  : 07/02/2014 9.19.54              Inj Volume : 10 µl

Acq. Method     : C:\HPCHEM\4\METHODS\NDI_095.M
Last changed    : 06/02/2014 14.00.34 by Nicola
                  (modified after loading)
Analysis Method : C:\HPCHEM\4\METHODS\EF.M
Last changed    : 04/06/2014 12.40.17 by Nicola
                  (modified after loading)
Sample Info     : NDI_102; AD-H 95/5 esano/ipa; 1 mL/min;
=====
```

=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.761	BV	0.2370	1337.27527	87.15366	7.2367
2	14.668	BB	0.3327	1.71417e4	791.30743	92.7633

Totals : 1.84790e4 878.46110

=====
*** End of Report ***

Data File S:\4\DATA\NDI\NDI_111_112_000.D
Sample Name: NDI_111_112

```
=====
Acq. Operator   : Nicola
Acq. Instrument : LC1100DAD                      Location : Vial 6
Injection Date  : 27/02/2014 11.27.08
                                           Inj Volume : 10 µl

Acq. Method     : C:\HPCHEM\4\METHODS\NDI_095.M
Last changed    : 07/02/2014 17.14.01 by Nicola
Analysis Method : C:\HPCHEM\4\METHODS\EF.M
Last changed    : 04/06/2014 12.40.17 by Nicola
                  (modified after loading)
Sample Info     : NDI_111_112; AD-H; 95/5 esano/ipa; 1 mL/min;
=====
```

=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.915	BB	0.2991	7912.19775	410.14478	54.1100
2	14.604	BB	0.3408	6710.24414	300.12491	45.8900

Totals : 1.46224e4 710.26968

=====
*** End of Report ***

Data File S:\4\DATA\NDI\NDI_111_000000.D
Sample Name: NDI_111

```
=====
Acq. Operator   : Nicola
Acq. Instrument : LC1100DAD                      Location : Vial 11
Injection Date  : 27/02/2014 11.49.13
                                           Inj Volume : 10 µl
Acq. Method     : C:\HPCHEM\4\METHODS\NDI_095.M
Last changed    : 07/02/2014 17.14.01 by Nicola
Analysis Method : C:\HPCHEM\4\METHODS\EF.M
Last changed    : 04/06/2014 12.40.17 by Nicola
                  (modified after loading)
Sample Info     : NDI_111; AD-H; 95/5 esano/ipa; 1 mL/min;
=====
```

=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.925	BB	0.2881	1.51893e4	805.23743	100.0000

Totals : 1.51893e4 805.23743

=====
*** End of Report ***

Data File S:\4\DATA\NDI\NDI_95_96_00006.D
Sample Name: NDI_95_96

```
=====
Acq. Operator   : Nicola
Acq. Instrument : LC1100DAD                      Location : Vial 91
Injection Date  : 06/02/2014 15.09.26
                                           Inj Volume : 10 µl

Acq. Method     : C:\HPCHEM\4\METHODS\NDI_095.M
Last changed    : 06/02/2014 14.00.34 by Nicola
                  (modified after loading)
Analysis Method : C:\HPCHEM\4\METHODS\EF.M
Last changed    : 04/06/2014 12.06.17 by Nicola
                  (modified after loading)
Sample Info     : NDI_95_96; AD-H 95/5 esano/ipa; 1 mL/min;
=====
```

=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 C, Sig=214,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.037	BB	0.3311	2.31783e4	1085.66663	58.9650
2	18.077	VB	0.4977	1.61302e4	482.92062	41.0350

Totals : 3.93085e4 1568.58725

=====
*** End of Report ***

Data File S:\4\DATA\NDI\NDI_095_000000.D
Sample Name: NDI_095

```
=====
Acq. Operator   : Nicola
Acq. Instrument : LC1100DAD                      Location : Vial 95
Injection Date  : 06/02/2014 17.19.39
                                           Inj Volume : 10 µl

Acq. Method     : C:\HPCHEM\4\METHODS\NDI_095.M
Last changed    : 06/02/2014 14.00.34 by Nicola
                  (modified after loading)
Analysis Method : C:\HPCHEM\4\METHODS\EF.M
Last changed    : 04/06/2014 12.22.54 by Nicola
                  (modified after loading)
Sample Info     : NDI_095; AD-H 95/5 esano/ipa; 1 mL/min;
=====
```

=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 C, Sig=214,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.151	BB	0.3281	2.11817e4	996.14771	100.0000

Totals : 2.11817e4 996.14771

=====
*** End of Report ***

Data File S:\4\DATA\NDI\NDI_096_000000.D
Sample Name: NDI_096

```
=====
Acq. Operator   : Nicola
Acq. Instrument : LC1100DAD                      Location : Vial 96
Injection Date  : 06/02/2014 18.05.37
                                           Inj Volume : 10 µl

Acq. Method     : C:\HPCHEM\4\METHODS\NDI_095.M
Last changed    : 06/02/2014 14.00.34 by Nicola
                  (modified after loading)
Analysis Method : C:\HPCHEM\4\METHODS\EF.M
Last changed    : 04/06/2014 12.22.54 by Nicola
                  (modified after loading)
Sample Info     : NDI_096; AD-H 95/5 esano/ipa; 1 mL/min;
=====
```

=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 C, Sig=214,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.159	BB	0.3210	646.92157	31.06118	4.1139
2	18.186	BB	0.5012	1.50782e4	447.38318	95.8861

Totals : 1.57251e4 478.44436

=====
*** End of Report ***

Data File S:\4\DATA\NDI\NDI_113_114_003.D
Sample Name: NDI_113_114

```
=====
Acq. Operator   : Nicola
Acq. Instrument : LC1100DAD                      Location : Vial 7
Injection Date  : 28/02/2014 13.56.44
                                           Inj Volume : 10 µl

Acq. Method     : C:\HPCHEM\4\METHODS\NDI_095.M
Last changed    : 28/02/2014 13.54.50 by Nicola
                  (modified after loading)
Analysis Method : C:\HPCHEM\4\METHODS\EF.M
Last changed    : 04/06/2014 13.46.41 by Nicola
                  (modified after loading)
Sample Info     : NDI_113_114; AD-H; 95/5 esano/ipa; 0.3 mL/min;
=====
```

=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	48.308	BB	0.8856	2.33362e4	405.37589	52.9060
2	55.733	VB	0.9980	2.07726e4	318.02353	47.0940

Totals : 4.41089e4 723.39941

=====
*** End of Report ***

Data File S:\4\DATA\NDI\NDI_113_000001.D
Sample Name: NDI_113_

```
=====
Acq. Operator   : Nicola
Acq. Instrument : LC1100DAD                      Location : Vial 13
Injection Date  : 28/02/2014 15.13.50
                                           Inj Volume : 10 µl

Acq. Method     : C:\HPCHEM\4\METHODS\NDI_095.M
Last changed    : 28/02/2014 13.54.50 by Nicola
                  (modified after loading)
Analysis Method : C:\HPCHEM\4\METHODS\EF.M
Last changed    : 04/06/2014 13.46.41 by Nicola
                  (modified after loading)
Sample Info     : NDI_113_; AD-H; 95/5 esano/ipa; 0.3 mL/min;
=====
```

```
=====
                        Area Percent Report
=====
```

```
Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Use Multiplier & Dilution Factor with ISTDs
```

Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	55.944	BB	1.0045	4.02593e4	619.21063	100.0000

Totals : 4.02593e4 619.21063

```
=====
*** End of Report ***
=====
```

Data File S:\4\DATA\NDI\NDI_114_000000.D
Sample Name: NDI_114

```
Acq. Operator   : Nicola
Acq. Instrument : LC1100DAD                      Location : Vial 14
Injection Date  : 28/02/2014 16.49.20
                                                    Inj Volume : 10 µl

Acq. Method     : C:\HPCHEM\4\METHODS\NDI_095.M
Last changed    : 28/02/2014 13.54.50 by Nicola
                  (modified after loading)
Analysis Method : C:\HPCHEM\4\METHODS\EF.M
Last changed    : 04/06/2014 13.46.41 by Nicola
                  (modified after loading)
Sample Info     : NDI_114; AD-H; 95/5 esano/ipa; 0.3 mL/min;
```

Area Percent Report

```
Sorted By      :      Signal
Multiplier    :      1.0000
Dilution      :      1.0000
Use Multiplier & Dilution Factor with ISTDs
```

Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	48.114	BB	0.8722	2.59946e4	460.73077	94.5541
2	55.371	VB	0.8962	1497.19116	24.45820	5.4459

Totals :	2.74918e4	485.18897
----------	-----------	-----------

*** End of Report ***

Data File S:\4\DATA\NDI\NDI_178_179_009.D
Sample Name: NDI_178_179

```
=====
Acq. Operator   : Nicola
Acq. Instrument : LC1100DAD                      Location : Vial 77
Injection Date  : 03/07/2014 11.21.06
                                           Inj Volume : 10 µl

Acq. Method     : C:\HPCHEM\4\METHODS\NDI_095.M
Last changed    : 03/07/2014 10.35.37 by Nicola
                  (modified after loading)
Analysis Method : C:\HPCHEM\4\METHODS\NDI_095.M
Last changed    : 03/07/2014 13.05.59 by Nicola
                  (modified after loading)
Sample Info     : NDI_178_179; amylose; Hex/IPA 95/5; 1 mL/min;
=====
```

=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.986	BB	0.5187	3437.71558	97.65135	27.4717
2	18.887	BB	0.9279	9075.94531	146.26830	72.5283

Totals : 1.25137e4 243.91965

=====
*** End of Report ***

Data File S:\4\DATA\NDI\NDI_178_000001.D
Sample Name: NDI_178

```
=====
Acq. Operator   : Nicola
Acq. Instrument : LC1100DAD                      Location : Vial 78
Injection Date  : 03/07/2014 11.49.38
                                           Inj Volume : 10 µl

Acq. Method     : C:\HPCHEM\4\METHODS\NDI_095.M
Last changed    : 03/07/2014 10.35.37 by Nicola
                  (modified after loading)
Analysis Method : C:\HPCHEM\4\METHODS\NDI_095.M
Last changed    : 03/07/2014 13.05.59 by Nicola
                  (modified after loading)
Sample Info     : NDI_178; amylose; Hex/IPA 95/5; 1 mL/min;
=====
```

=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.200	BB	0.4813	236.49847	7.31268	1.4544
2	18.745	BB	0.9803	1.60246e4	243.33011	98.5456

Totals : 1.62611e4 250.64279

=====
*** End of Report ***

Data File S:\4\DATA\NDI\NDI_179_000000.D
Sample Name: NDI_179

```
=====
Acq. Operator   : Nicola
Acq. Instrument : LC1100DAD                      Location : Vial 79
Injection Date  : 03/07/2014 12.15.40
                                           Inj Volume : 10 µl

Acq. Method     : C:\HPCHEM\4\METHODS\NDI_095.M
Last changed    : 03/07/2014 10.35.37 by Nicola
                  (modified after loading)
Analysis Method : C:\HPCHEM\4\METHODS\NDI_095.M
Last changed    : 03/07/2014 13.05.59 by Nicola
                  (modified after loading)
Sample Info     : NDI_179; amylose; Hex/IPA 95/5; 1 mL/min;
=====
```

```
=====
                        Area Percent Report
=====
```

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.967	BB	0.5032	5006.36377	144.85658	97.9929
2	19.219	MM	1.2003	102.54273	1.42386	2.0071

Totals : 5108.90650 146.28044

```
=====
*** End of Report ***
=====
```

Data File S:\4\DATA\NDI\NDI_137_138A_00.D
Sample Name: NDI_137_138A

```
=====
Acq. Operator   : NDI
Acq. Instrument : LC1100DAD                      Location : Vial 35
Injection Date  : 09/04/2014 14.38.58
                                           Inj Volume : 10 µl

Acq. Method     : C:\HPCHEM\4\METHODS\NDI_095.M
Last changed    : 09/04/2014 13.58.09 by NDI
                  (modified after loading)
Analysis Method : C:\HPCHEM\4\METHODS\EF.M
Last changed    : 04/06/2014 13.46.41 by Nicola
                  (modified after loading)
Sample Info     : NDI_137_138A; AD-H; Hex/IPA 95/5; 0.5 mL/min
=====
```

=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	22.255	BB	0.4046	1.42500e4	542.32526	57.1507
2	24.308	BB	0.4478	1.06841e4	366.85291	42.8493

Totals : 2.49341e4 909.17816

=====
*** End of Report ***

Data File S:\4\DATA\NDI\NDI_137_000000.D
Sample Name: NDI_137

```
=====
Acq. Operator   : NDI
Acq. Instrument : LC1100DAD                      Location : Vial 37
Injection Date  : 09/04/2014 16.26.21
                                           Inj Volume : 10 µl

Acq. Method     : C:\HPCHEM\4\METHODS\NDI_095.M
Last changed    : 09/04/2014 13.58.09 by NDI
                  (modified after loading)
Analysis Method : C:\HPCHEM\4\METHODS\EF.M
Last changed    : 04/06/2014 13.46.41 by Nicola
                  (modified after loading)
Sample Info     : NDI_137; AD-H; Hex/IPA 95/5; 0.5 mL/min
=====
```

```
=====
                        Area Percent Report
=====
```

```
Sorted By      : Signal
Multiplier     : 1.0000
Dilution       : 1.0000
Use Multiplier & Dilution Factor with ISTDs
```

Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	22.357	BB	0.4031	2.67553e4	1029.75439	100.0000

Totals : 2.67553e4 1029.75439

```
=====
*** End of Report ***
=====
```



```
=====
Acq. Operator   : NDI
Acq. Instrument : LC1100DAD                      Location : Vial 47
Injection Date  : 09/04/2014 17.37.17
                                           Inj Volume : 10 µl
Acq. Method     : C:\HPCHEM\4\METHODS\NDI_095.M
Last changed    : 09/04/2014 13.58.09 by NDI
                  (modified after loading)
Analysis Method : C:\HPCHEM\4\METHODS\EF.M
Last changed    : 04/06/2014 13.46.41 by Nicola
                  (modified after loading)
Sample Info     : NDI_138A; AD-H; Hex/IPA 95/5; 0.5 mL/min
=====
```

```
Sorted By      :      Signal
Multiplier    :      1.0000
Dilution      :      1.0000
Use Multiplier & Dilution Factor with ISTDs
```

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	22.364	BB	0.4106	1443.67676	53.19787	6.3647
2	24.317	BB	0.4576	2.12389e4	717.01544	93.6353

*** End of Report ***

Data File S:\4\DATA\NDI\NDI139_40_41_13.D
Sample Name: NDI_139_40_41

```
=====
Acq. Operator   : Nicola
Acq. Instrument : LC1100DAD                      Location : Vial 38
Injection Date  : 04/06/2014 15.45.21
                                           Inj Volume : 10 µl

Acq. Method     : C:\HPCHEM\4\METHODS\EF.M
Last changed    : 04/06/2014 15.39.39 by Nicola
                  (modified after loading)
Analysis Method : C:\HPCHEM\4\METHODS\EF.M
Last changed    : 05/06/2014 11.55.37 by Nicola
                  (modified after loading)
Sample Info     : NDI_139_40_41; cellulose; 90/10 Hex/IPA; 0.5 mL/min
=====
```

=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 C, Sig=214,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	39.289	FM	1.5700	5785.98340	61.42150	24.1835
2	43.168	FM	3.6828	1.81394e4	82.08984	75.8165

Totals : 2.39253e4 143.51135

=====
*** End of Report ***

Data File S:\4\DATA\NDI\NDI_140_000003.D
Sample Name: NDI_140

```
=====
Acq. Operator   : Nicola
Acq. Instrument : LC1100DAD                      Location : Vial 40
Injection Date  : 04/06/2014 18.00.57
                                           Inj Volume : 10 µl

Acq. Method     : C:\HPCHEM\4\METHODS\EF.M
Last changed    : 04/06/2014 15.39.39 by Nicola
                  (modified after loading)
Analysis Method : C:\HPCHEM\4\METHODS\EF.M
Last changed    : 05/06/2014 11.55.37 by Nicola
                  (modified after loading)
Sample Info     : NDI_140; cellulose; 90/10 Hex/IPA; 0.5 mL/min
=====
```

```
=====
                          Area Percent Report
=====
```

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 C, Sig=214,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	38.794	BB	1.4164	5.38206e4	569.60449	100.0000

Totals : 5.38206e4 569.60449

```
=====
*** End of Report ***
=====
```

Data File S:\4\DATA\NDI\NDI_145_46A_001.D
Sample Name: NDI_145_46A

```
=====
Acq. Operator   : Nicola
Acq. Instrument : LC1100DAD                      Location : Vial 43
Injection Date  : 22/04/2014 15.41.06
                                           Inj Volume : 10 µl

Acq. Method     : C:\HPCHEM\4\METHODS\NDI_095.M
Last changed    : 22/04/2014 15.06.32 by Nicola
                  (modified after loading)
Analysis Method : C:\HPCHEM\4\METHODS\EF.M
Last changed    : 04/06/2014 13.46.41 by Nicola
                  (modified after loading)
Sample Info     : NDI_145_46A; AD-H; Hex/IPA 95/5; 0.5 mL/min
=====
```

=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	46.234	BB	0.8661	1.04740e4	189.72238	44.1674
2	49.598	BB	0.9084	1.32403e4	223.08711	55.8326

Totals : 2.37142e4 412.80949

=====
*** End of Report ***

Data File S:\4\DATA\NDI\NDI_145_000000.D
Sample Name: NDI_145

```
=====
Acq. Operator   : Nicola
Acq. Instrument : LC1100DAD                      Location : Vial 45
Injection Date  : 22/04/2014 16.54.37
                                           Inj Volume : 10 µl

Acq. Method     : C:\HPCHEM\4\METHODS\NDI_095.M
Last changed    : 22/04/2014 15.06.32 by Nicola
                  (modified after loading)
Analysis Method : C:\HPCHEM\4\METHODS\EF.M
Last changed    : 04/06/2014 13.46.41 by Nicola
                  (modified after loading)
Sample Info     : NDI_145; AD-H; Hex/IPA 95/5; 0.5 mL/min
=====
```

```
=====
                        Area Percent Report
=====
```

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	49.276	BB	0.9098	2.60662e4	439.58154	100.0000

Totals : 2.60662e4 439.58154

```
=====
*** End of Report ***
=====
```

Data File S:\4\DATA\NDI\NDI_146B_000000.D
Sample Name: NDI_146B

```
=====
Acq. Operator   : Nicola
Acq. Instrument : LC1100DAD                      Location : Vial 55
Injection Date  : 22/04/2014 17.57.31
                                           Inj Volume : 10 µl

Acq. Method     : C:\HPCHEM\4\METHODS\NDI_095.M
Last changed    : 22/04/2014 15.06.32 by Nicola
                  (modified after loading)
Analysis Method : C:\HPCHEM\4\METHODS\EF.M
Last changed    : 04/06/2014 14.54.37 by Nicola
                  (modified after loading)
Sample Info     : NDI_146B; AD-H; Hex/IPA 95/5; 0.5 mL/min
=====
```

=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	46.163	BB	0.8498	2.09797e4	379.01410	100.0000

Totals : 2.09797e4 379.01410

=====
*** End of Report ***

Data File S:\4\DATA\NDI\NDI_176_177_000.D
Sample Name: NDI_176_177

```
=====
Acq. Operator   : Nicola
Acq. Instrument : LC1100DAD                      Location : Vial 75
Injection Date  : 01/07/2014 14.27.49
                                           Inj Volume : 10 µl

Acq. Method     : C:\HPCHEM\4\METHODS\NDI_095.M
Last changed    : 01/07/2014 13.44.34 by claudio
                  (modified after loading)
Analysis Method : C:\HPCHEM\4\METHODS\NDI_095.M
Last changed    : 07/05/2014 14.32.35 by Nicola
Sample Info     : NDI_176_177; AD-H; Hex/IPA 90/10; 1 mL/min;
=====
```

=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 C, Sig=214,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.710	BB	0.3787	2.30281e4	950.50824	47.2456
2	24.794	BB	0.5715	2.57132e4	701.73676	52.7544

Totals : 4.87413e4 1652.24500

=====
*** End of Report ***

Data File S:\4\DATA\NDI\NDI_176_000000.D
Sample Name: NDI_176

```
=====
Acq. Operator   : Nicola
Acq. Instrument : LC1100DAD                      Location : Vial 76
Injection Date  : 01/07/2014 15.00.51
                                           Inj Volume : 10 µl

Acq. Method     : C:\HPCHEM\4\METHODS\NDI_095.M
Last changed    : 01/07/2014 13.44.34 by claudio
                  (modified after loading)
Analysis Method : C:\HPCHEM\4\METHODS\NDI_095.M
Last changed    : 07/05/2014 14.32.35 by Nicola
Sample Info     : NDI_176; AD-H; Hex/IPA 90/10; 1 mL/min;
=====
```

=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 C, Sig=214,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.691	BB	0.3707	70.08877	2.95471	0.1473
2	24.620	VB	0.5973	4.75074e4	1255.89661	99.8527

Totals : 4.75775e4 1258.85131

=====
*** End of Report ***

Data File S:\4\DATA\NDI\NDI_177_000000.D
Sample Name: NDI_177

```
=====
Acq. Operator   : Nicola
Acq. Instrument : LC1100DAD                      Location : Vial 77
Injection Date  : 01/07/2014 15.36.26
                                           Inj Volume : 10 µl
Acq. Method     : C:\HPCHEM\4\METHODS\NDI_095.M
Last changed    : 01/07/2014 13.44.34 by claudio
                  (modified after loading)
Analysis Method : C:\HPCHEM\4\METHODS\NDI_095.M
Last changed    : 07/05/2014 14.32.35 by Nicola
Sample Info     : NDI_177; AD-H; Hex/IPA 90/10; 1 mL/min;
=====
```

=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 C, Sig=214,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.360	BB	0.4209	4.15418e4	1568.91895	99.3802
2	24.260	BB	0.5515	259.08331	7.13697	0.6198

Totals : 4.18009e4 1576.05591

=====
*** End of Report ***

Data File S:\4\DATA\NDI\NDI_115_116_000.D
Sample Name: NDI_115_116

```
=====
Acq. Operator   : Nicola
Acq. Instrument : LC1100DAD                      Location : Vial 8
Injection Date  : 28/02/2014 12.44.14
                                           Inj Volume : 10 µl

Acq. Method     : C:\HPCHEM\4\METHODS\NDI_095.M
Last changed    : 28/02/2014 12.42.31 by Nicola
                  (modified after loading)
Analysis Method : C:\HPCHEM\4\METHODS\EF.M
Last changed    : 04/06/2014 13.46.41 by Nicola
                  (modified after loading)
Sample Info     : NDI_115_116; AD-H; 95/5 esano/ipa; 1 mL/min;
=====
```

```
=====
                          Area Percent Report
=====
```

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.997	VV	0.1168	8676.79687	1114.65320	61.7801
2	10.648	BV	0.2466	5367.84766	335.59384	38.2199

Totals : 1.40446e4 1450.24704

```
=====
*** End of Report ***
=====
```

Data File S:\4\DATA\NDI\NDI_115_000000.D
Sample Name: NDI_115

```
=====
Acq. Operator   : Nicola
Acq. Instrument : LC1100DAD                      Location : Vial 15
Injection Date  : 28/02/2014 12.58.12
                                           Inj Volume : 10 µl

Acq. Method     : C:\HPCHEM\4\METHODS\NDI_095.M
Last changed    : 28/02/2014 12.42.31 by Nicola
                  (modified after loading)
Analysis Method : C:\HPCHEM\4\METHODS\EF.M
Last changed    : 04/06/2014 13.46.41 by Nicola
                  (modified after loading)
Sample Info     : NDI_115; AD-H; 95/5 esano/ipa; 1 mL/min;
=====
```

Area Percent Report

```
Sorted By      : Signal
Multiplier     : 1.0000
Dilution       : 1.0000
Use Multiplier & Dilution Factor with ISTDs
```

Signal 1: DAD1 C, Sig=214,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.048	MM	0.1169	105.58023	15.05258	0.3081
2	10.659	BB	0.2950	3.41661e4	1837.13257	99.6919

Totals : 3.42717e4 1852.18515

*** End of Report ***

Data File S:\4\DATA\NDI\NDI_116_000000.D
Sample Name: NDI_116

```
=====
Acq. Operator   : Nicola
Acq. Instrument : LC1100DAD                      Location : Vial 16
Injection Date  : 28/02/2014 13.41.24
                                           Inj Volume : 10 µl

Acq. Method     : C:\HPCHEM\4\METHODS\NDI_095.M
Last changed    : 28/02/2014 12.42.31 by Nicola
                  (modified after loading)
Analysis Method : C:\HPCHEM\4\METHODS\EF.M
Last changed    : 04/06/2014 13.46.41 by Nicola
                  (modified after loading)
Sample Info     : NDI_116; AD-H; 95/5 esano/ipa; 1 mL/min;
=====
```

=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 C, Sig=214,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.000	VV	0.1878	2.36800e4	2064.13281	86.5367
2	11.248	VB	0.2346	3684.12085	230.31244	13.4633

Totals : 2.73642e4 2294.44525

=====
*** End of Report ***

Data File S:\4\DATA\NDI\NDI_53_54_RAC_0.D
Sample Name: NDI_53_54_rac

```
=====
Acq. Operator   : Nicola
Acq. Instrument : LC1100DAD                      Location : Vial 56
Injection Date  : 18/07/2013 22.34.34
                                           Inj Volume : 5 µl

Acq. Method     : S:\4\METHODS\NDI\NDI_016_B.M
Last changed    : 13/06/2013 13.55.39 by Nicola
Analysis Method : C:\HPCHEM\4\METHODS\EF.M
Last changed    : 04/06/2014 12.06.17 by Nicola
                  (modified after loading)
Sample Info     : NDI_53_54_rac; AD-H; esano/ipa 90/10; 0.5 mL/min;
=====
```

Area Percent Report

```
=====
Sorted By      : Signal
Multiplier     : 1.0000
Dilution       : 1.0000
Use Multiplier & Dilution Factor with ISTDs
=====
```

Signal 1: DAD1 C, Sig=214,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.174	BB	0.2718	5233.44531	293.83963	61.9839
2	22.784	BB	0.4146	3209.78979	119.02245	38.0161

Totals : 8443.23511 412.86208

*** End of Report ***

Data File S:\4\DATA\NDI\NDI_053_000000.D
Sample Name: NDI_053

```
=====
Acq. Operator   : Nicola
Acq. Instrument : LC1100DAD                      Location : Vial 53
Injection Date  : 18/07/2013 23.16.18
                                           Inj Volume : 5 µl

Acq. Method     : S:\4\METHODS\NDI\NDI_016_B.M
Last changed    : 13/06/2013 13.55.39 by Nicola
Analysis Method : C:\HPCHEM\4\METHODS\EF.M
Last changed    : 04/06/2014 12.06.17 by Nicola
                  (modified after loading)
Sample Info     : NDI_053; AD-H; esano/ipa 90/10; 0.5 mL/min;
=====
```

=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 C, Sig=214,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.158	BB	0.2735	1.12174e4	630.63947	100.0000

Totals : 1.12174e4 630.63947

=====
*** End of Report ***

Data File S:\4\DATA\NDI\NDI_054_000000.D
Sample Name: NDI_054

```
=====
Acq. Operator   : Nicola
Acq. Instrument : LC1100DAD                      Location : Vial 54
Injection Date  : 18/07/2013 23.53.11
                                           Inj Volume : 5 µl

Acq. Method     : S:\4\METHODS\NDI\NDI_016_B.M
Last changed    : 13/06/2013 13.55.39 by Nicola
Analysis Method : C:\HPCHEM\4\METHODS\EF.M
Last changed    : 04/06/2014 12.06.17 by Nicola
                  (modified after loading)
Sample Info     : NDI_054; AD-H; esano/ipa 90/10; 0.5 mL/min;
=====
```

=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 C, Sig=214,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.168	BB	0.2939	207.68193	10.54110	3.7365
2	22.775	VB	0.4198	5350.52783	197.66032	96.2635

Totals : 5558.20976 208.20142

=====
*** End of Report ***

Compound (Z)-4n, conformer a

Method: **b3lyp/6-311++g(2d,p)**

SCF Done: E(RB3LYP) = -1757.84526889

A.U. after

1 cycles

Lowest frequency = 16.6083

Zero-point correction= 0.368324
(Hartree/Particle)
Thermal correction to Energy= 0.395029
Thermal correction to Enthalpy= 0.395973
Thermal correction to Gibbs Free Energy= 0.306432
Sum of electronic and zero-point Energies= -1757.476945
Sum of electronic and thermal Energies= -1757.450240
Sum of electronic and thermal Enthalpies= -1757.449296
Sum of electronic and thermal Free Energies= -1757.538837

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)			
Number	Number	Type	X	Y	Z	

1	1	0	2.052674	-3.227169	-	0.647707
2	6	0	2.663124	-2.357384	-	0.465343
3	6	0	4.325946	-0.141470	-	0.031683
4	6	0	2.110315	-1.078489	-	0.421215
5	6	0	4.028339	-2.538137	-	0.266437
6	6	0	4.834408	-1.435947	-	0.025029
7	6	0	2.963885	0.012886	-	0.167967
8	1	0	4.964514	0.701843	-	0.232115
9	6	0	0.747882	-0.570654	-	0.597810
10	6	0	0.824318	0.908761	-	0.370425
11	7	0	2.207480	1.213244	-	0.170204
12	8	0	-0.073713	1.713105	-	0.311393
13	6	0	-0.393218	-1.223047	-	0.935669

14	6	0	-0.412154	-2.715342	-
1.139735					
15	1	0	-0.104580	-3.251619	-
0.238075					
16	1	0	0.271136	-3.010602	-
1.941544					
17	1	0	-1.409160	-3.061373	-
1.410109					
18	6	0	-1.715032	-0.536043	-
1.168219					
19	1	0	-2.151561	-0.967657	-
2.074232					
20	1	0	-1.584038	0.528480	-
1.332872					
21	6	0	-2.752958	-0.765091	-
0.028314					
22	1	0	-2.808136	-1.835700	
0.177894					
23	6	0	-4.137232	-0.300875	-
0.449538					
24	6	0	-6.699014	0.519463	-
1.241869					
25	6	0	-5.195679	-1.208577	-
0.493461					
26	6	0	-4.382754	1.028682	-
0.804790					
27	6	0	-5.651958	1.435367	-
1.198164					
28	6	0	-6.467749	-0.804049	-
0.887305					
29	1	0	-5.025731	-2.240558	-
0.207179					
30	1	0	-3.579754	1.756803	-
0.775640					
31	1	0	-5.824197	2.470257	-
1.469199					
32	1	0	-7.277406	-1.523723	-
0.911289					
33	1	0	-7.688693	0.837782	-
1.546795					
34	6	0	2.768322	2.482181	
0.052959					
35	8	0	3.905872	2.642919	
0.424166					
36	8	0	1.908185	3.460633	-
0.214046					
37	6	0	2.409507	4.792055	
0.015902					
38	1	0	1.579497	5.449108	-
0.227699					
39	1	0	3.264379	4.991408	-
0.628846					

40	1	0	2.703929	4.911000	
1.057597					
41	6	0	-2.284103	-0.090409	
1.265579					
42	1	0	-1.268747	-0.395137	
1.521376					
43	1	0	-2.340958	0.992335	
1.233490					
44	7	0	-3.119167	-0.523606	
2.448164					
45	8	0	-3.279695	-1.726550	
2.610192					
46	8	0	-3.558387	0.349351	
3.179001					
47	17	0	6.554453	-1.671931	
0.223951					
48	1	0	4.459692	-3.529068	-
0.296534					

Compound (Z)-4n, conformer b

Method: **b3lyp/6-311++g(2d,p)**

SCF Done: E(RB3LYP) = -1757.84503264 A.U. after 1 cycles

Lowest frequency = 17.7177

Zero-point correction=	0.368469
(Hartree/Particle)	
Thermal correction to Energy=	0.395040
Thermal correction to Enthalpy=	0.395984
Thermal correction to Gibbs Free Energy=	0.307646
Sum of electronic and zero-point Energies=	-1757.476563
Sum of electronic and thermal Energies=	-1757.449993
Sum of electronic and thermal Enthalpies=	-1757.449048
Sum of electronic and thermal Free Energies=	-1757.537387

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	1.899415	-3.126952	-
0.798930					
2	6	0	2.482948	-2.236402	-
0.629899					

3	6	0	4.075010	0.035458	-
0.154504					
4	6	0	1.880502	-0.984664	-
0.518262					
5	6	0	3.863468	-2.362356	-
0.511847					
6	6	0	4.633711	-1.232928	-
0.281352					
7	6	0	2.698592	0.134973	-
0.274516					
8	1	0	4.334082	-3.332263	-
0.594203					
9	1	0	4.687287	0.899825	
0.036773					
10	6	0	0.490330	-0.534370	-
0.606858					
11	6	0	0.513928	0.938809	-
0.332298					
12	7	0	1.890375	1.299240	-
0.189415					
13	8	0	-0.413159	1.704495	-
0.216677					
14	6	0	-0.634574	-1.230406	-
0.909718					
15	6	0	-0.595647	-2.711549	-
1.176745					
16	1	0	-0.235760	-3.264788	-
0.306257					
17	1	0	0.067357	-2.942026	-
2.015899					
18	1	0	-1.587437	-3.089913	-
1.422625					
19	6	0	-1.994589	-0.592491	-
1.044657					
20	1	0	-2.464962	-1.014738	-
1.938420					
21	1	0	-1.906266	0.479416	-
1.187249					
22	6	0	-2.971877	-0.863179	
0.137047					
23	1	0	-3.087380	-1.940550	
0.265331					
24	6	0	-4.344208	-0.284625	-
0.173696					
25	6	0	-6.889028	0.752881	-
0.739037					
26	6	0	-5.451269	-1.126962	-
0.284302					
27	6	0	-4.531483	1.089485	-
0.352254					
28	6	0	-5.793145	1.603477	-
0.630103					

29	6	0	-6.714399	-0.615263	-
0.566294					
30	1	0	-5.324861	-2.195654	-
0.147683					
31	1	0	-3.688517	1.767402	-
0.278286					
32	1	0	-5.919682	2.671394	-
0.763439					
33	1	0	-7.560540	-1.287047	-
0.649872					
34	1	0	-7.871172	1.154455	-
0.957782					
35	6	0	2.407044	2.581862	
0.053251					
36	8	0	3.569624	2.787055	
0.307447					
37	8	0	1.475012	3.526603	-
0.049791					
38	6	0	1.939173	4.866282	
0.203574					
39	1	0	1.057856	5.492410	
0.095990					
40	1	0	2.703835	5.146570	-
0.519758					
41	1	0	2.346912	4.942484	
1.210578					
42	6	0	-2.474519	-0.306678	
1.477554					
43	1	0	-2.043856	0.687410	
1.403162					
44	1	0	-3.284072	-0.298449	
2.209109					
45	7	0	-1.410139	-1.159918	
2.141390					
46	8	0	-1.484089	-2.375264	
2.014762					
47	8	0	-0.571780	-0.575683	
2.808319					
48	17	0	6.374789	-1.399413	-
0.136902					

Compound (Z)-4n, conformer d

Method: **b3lyp/6-311++g(2d,p)**

SCF Done: E(RB3LYP) = -1757.84466656 A.U. after 1 cycles

Lowest frequency = 10.0600

Zero-point correction= 0.368276
 (Hartree/Particle)
 Thermal correction to Energy= 0.394996
 Thermal correction to Enthalpy= 0.395941
 Thermal correction to Gibbs Free Energy= 0.305492
 Sum of electronic and zero-point Energies= -1757.476390
 Sum of electronic and thermal Energies= -1757.449670
 Sum of electronic and thermal Enthalpies= -1757.448726
 Sum of electronic and thermal Free Energies= -1757.539174

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)			
Number	Number	Type	X	Y	Z	

1	1	0	-1.267654	-3.226154	-	
0.501102						
2	6	0	-1.983767	-2.425492	-	
0.409875						
3	6	0	-3.909682	-0.397403	-	
0.107959						
4	6	0	-1.594636	-1.089864	-	
0.498533						
5	6	0	-3.316866	-2.755442	-	
0.185532						
6	6	0	-4.254320	-1.744174	-	
0.044215						
7	6	0	-2.576283	-0.094178	-	
0.332733						
8	1	0	-4.648018	0.375557		
0.017764						
9	6	0	-0.298606	-0.439244	-	
0.708654						
10	6	0	-0.555643	1.035499	-	
0.617704						
11	7	0	-1.969069	1.185001	-	
0.425009						
12	8	0	0.222838	1.953807	-	
0.690076						
13	6	0	0.910134	-0.988744	-	
0.986249						
14	6	0	1.073949	-2.474464	-	
1.173647						
15	1	0	0.322333	-2.871163	-	
1.859119						
16	1	0	0.969121	-3.013556	-	
0.226568						
17	1	0	2.056083	-2.711448	-	
1.581973						

18	6	0	2.176450	-0.191025	-
1.163237					
19	1	0	1.973289	0.874523	-
1.161644					
20	1	0	2.580739	-0.450764	-
2.149184					
21	6	0	3.262357	-0.532425	-
0.108027					
22	1	0	3.487184	-1.598440	-
0.163756					
23	6	0	2.868230	-0.220350	
1.328379					
24	6	0	2.241233	0.323352	
4.008584					
25	6	0	3.045275	-1.190938	
2.316904					
26	6	0	2.369561	1.029717	
1.703673					
27	6	0	2.060011	1.298228	
3.032808					
28	6	0	2.733565	-0.925283	
3.646433					
29	1	0	3.431817	-2.167290	
2.043584					
30	1	0	2.196721	1.795306	
0.957475					
31	1	0	1.671615	2.272655	
3.304489					
32	1	0	2.874480	-1.694334	
4.396698					
33	1	0	1.996583	0.534459	
5.042692					
34	6	0	-2.686600	2.387402	-
0.326167					
35	8	0	-3.870678	2.430204	-
0.090102					
36	8	0	-1.916942	3.453592	-
0.531322					
37	6	0	-2.599276	4.719347	-
0.447288					
38	1	0	-3.387348	4.776320	-
1.196936					
39	1	0	-1.831123	5.463717	-
0.637375					
40	1	0	-3.031229	4.853026	
0.543609					
41	6	0	4.569856	0.204208	-
0.429334					
42	1	0	4.446402	1.281535	-
0.501511					
43	1	0	5.334582	-0.030623	
0.311538					

44	7	0	5.164103	-0.233043	-
1.750552					
45	8	0	5.263807	-1.436663	-
1.948909					
46	8	0	5.520511	0.640138	-
2.525850					
47	1	0	-3.621101	-3.790792	-
0.117553					
48	17	0	-5.934451	-2.166895	
0.236007					

Compound (Z)-4n, conformer d

Method: **b3lyp/6-311++g(2d,p)**

SCF Done: E(RB3LYP) = -1757.84426118 A.U. after 1 cycles

Lowest frequency = 15.1279

Zero-point correction=	0.368332
(Hartree/Particle)	
Thermal correction to Energy=	0.395013
Thermal correction to Enthalpy=	0.395957
Thermal correction to Gibbs Free Energy=	0.306390
Sum of electronic and zero-point Energies=	-1757.475930
Sum of electronic and thermal Energies=	-1757.449248
Sum of electronic and thermal Enthalpies=	-1757.448304
Sum of electronic and thermal Free Energies=	-1757.537871

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	1.494067	-3.156646	-
0.764778					
2	6	0	2.203281	-2.394853	-
0.482886					
3	6	0	4.108694	-0.466815	
0.277514					
4	6	0	1.850688	-1.046499	-
0.468509					
5	6	0	3.489746	-2.786163	-
0.124896					
6	6	0	4.416878	-1.823728	
0.245534					

7	6	0	2.821861	-0.101399	-
0.083130					
8	1	0	3.766849	-3.831289	-
0.132018					
9	1	0	4.838287	0.266043	
0.577047					
10	6	0	0.613941	-0.334189	-
0.789930					
11	6	0	0.886668	1.113421	-
0.533103					
12	7	0	2.262661	1.201146	-
0.145524					
13	8	0	0.125331	2.048053	-
0.598603					
14	6	0	-0.571948	-0.796590	-
1.261562					
15	6	0	-0.800068	-2.263347	-
1.507971					
16	1	0	-0.671145	-2.844497	-
0.590989					
17	1	0	-0.089966	-2.653960	-
2.243661					
18	1	0	-1.806858	-2.449506	-
1.875968					
19	6	0	-1.726210	0.124623	-
1.573081					
20	1	0	-2.341552	-0.336393	-
2.349546					
21	1	0	-1.349708	1.071892	-
1.954127					
22	6	0	-2.618686	0.428928	-
0.330929					
23	1	0	-1.958832	0.719188	
0.485437					
24	6	0	-3.443586	-0.765878	
0.118354					
25	6	0	-4.929317	-2.990516	
0.968650					
26	6	0	-3.199304	-1.357609	
1.358009					
27	6	0	-4.453052	-1.303082	-
0.685676					
28	6	0	-5.190364	-2.404074	-
0.266184					
29	6	0	-3.932228	-2.462832	
1.780406					
30	1	0	-2.434296	-0.941645	
2.003777					
31	1	0	-4.675179	-0.860120	-
1.650684					
32	1	0	-5.972307	-2.801941	-
0.902157					

33	1	0	-3.727672	-2.905139	
2.748209					
34	1	0	-5.504798	-3.847467	
1.297527					
35	6	0	-3.470998	1.656964	-
0.663640					
36	1	0	-2.825041	2.508790	-
0.881247					
37	1	0	-4.163772	1.498832	-
1.485961					
38	7	0	-4.322040	2.101991	
0.502557					
39	8	0	-3.783557	2.172943	
1.596473					
40	8	0	-5.487503	2.385368	
0.267943					
41	17	0	6.036958	-2.325423	
0.695669					
42	6	0	2.976220	2.365860	
0.180496					
43	8	0	4.080052	2.346843	
0.670095					
44	8	0	2.300674	3.468693	-
0.130721					
45	6	0	2.966009	4.703588	
0.198428					
46	1	0	3.903528	4.786807	-
0.349701					
47	1	0	2.271926	5.483495	-
0.101683					
48	1	0	3.164505	4.753738	
1.268050					

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