Supporting Information

Damage Incorporated: Discovery of the Potent, Highly Selective, Orally Available ATR Inhibitor BAY 1895344 with Favorable Pharmacokinetic Properties and Promising Efficacy in Monotherapy and in Combination Treatments in Preclinical Tumor Models

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Kinase Selectivity Panel Data for BAY 1895344

Table S1. DiscoverX kinase selectivity panel performed at 100 nM and 1000 nM compound concentration. The results are sorted ascendingly for % of control at 1000 nM compound concentration. K_D values were determined for all off-target hits <50% (see Figure S1 below).

DiscoverX Gene Symbol	% Control @ 100 nM	% Control @ 1000 nM
MTOR	41	2.2
DYRK1B	28	11
VPS34	46	17
RIOK2	93	24
GAK	85	27
GSK3A	54	31
DDR1	36	36
PIK3CA(I800L)	79	36
CSNK2A2	43	38
ACVRL1	79	41
PIKFYVE	89	51
PIK3C2G	90	51
WNK4	53	53
GRK7	59	55
AXL	56	56
TESK1	64	56
MYLK2	82	56
PIK3CB	96	57
TXK	67	58
PIK3CG	75	58
WNK3	75	58
MAST1	89	59
ZAK	66	61
TYRO3	73	62
NDR2	70	63
WNK1	78	63
FGFR3(G697C)	60	64
TGFBR1	56	65
MLK2	74	65
PRKG1	100	65
PIK3CA(E545K)	86	67
MERTK	71	68
FLT3(K663Q)	87	68
MST2	52	69
RET(V804M)	92	69
MAP3K4	81	71
ABL1(Q252H)-nonphosphorylated	82	72

FLT3(D835Y)	100	72
RAF1	63	73
JAK3(JH1domain-catalytic)	78	73
RIPK4	81	73
TNK1	83	73
ABL1-nonphosphorylated	89	73
FLT3(D835H)	57	74
CSNK1D	74	74
ABL1(H396P)-nonphosphorylated	79	74
LZK	89	74
RSK3(Kin.Dom.1-N-terminal)	92	74
TRKA	100	74
PKNB(M.tuberculosis)	65	75
LATS2	88	75
CDK8	77	76
CASK	79	76
ACVR1	100	76
FLT3(N841I)	62	77
EPHA1	71	77
PCTK2	73	77
BRAF	100	77
PIK3CD	94	78
AKT3	100	78
RPS6KA4(Kin.Dom.1-N-terminal)	100	78
KIT(L576P)	49	79
ASK2	84	79
MARK2	87	79
TIE2	91	79
p38-gamma	93	79
CIT	100	79
RET(M918T)	64	80
MAK	77	81
MELK	78	81
ACVR1B	89	81
PIK3CA(E542K)	83	82
ABL1(F317I)-nonphosphorylated	90	82
MEK5	94	82
MAP3K1	75	83
CSF1R-autoinhibited	80	83
PRKCD	84	83
SRPK1	85	83
BLK	94	83
ICK	95	83
BMPR1A	100	83
PDGFRB	65	84
PAK4	70	84
MLCK	71	84
ERBB3	72	84
CDKL1	83	84

FGR	84	84
BMPR1B	94	84
CLK2	94	84
GRK4	100	84
ROS1	100	84
CDK2	79	85
FES	80	85
JNK1	93	85
WEE2	70	86
EGFR(T790M)	77	86
YANK1	84	86
MARK3	89	86
MEK6	90	86
PIK4CB	91	86
PLK1	91	86
EPHA6	93	86
EIF2AK1	95	86
NEK3	100	86
PRKCQ	86	87
p38-beta	87	87
SGK	90	87
ABL1(T315I)-nonphosphorylated	91	87
JNK2	97	87
EPHB1	100	87
PIK3C2B	100	87
BIKE	65	88
STK16	72	88
NEK9	73	88
SRPK2	78	88
YANK3	78	88
MARK1	84	88
AKT2	85	88
FGFR1	89	88
MKK7	100	88
MET(M1250T)	72	89
CSNK1A1L	77	89
DAPK2	78	89
DLK	79	89
BUB1	92	89
ULK1	97	89
MST1R	100	89
BRK	79	90
PCTK3	82	90
JAK1(JH1domain-catalytic)	84	90
VRK2	86	90
ROCK1	88	90
CHEK1	89	90
HIPK1	90	90
NIM1	90	90

ERK4	91	90
PIK3CA(Q546K)	98	90
CDKL2	99	90
LRRK2(G2019S)	78	91
PRKD3	82	91
INSR	83	91
WNK2	84	91
EPHB3	95	91
MAP3K2	100	91
PRKCH	100	91
TBK1	100	91
TSSK3	100	91
CAMK1	56	92
TTK	65	92
CAMK2A	83	92
HPK1	87	92
ABL1(F317L)-nonphosphorylated	91	92
CAMK1B	95	92
ABL1-phosphorylated	98	92
HIPK4	98	92
NDR1	98	92
MAP4K5	99	92
CSNK1A1	100	92
KIT	73	93
EPHA5	83	93
PAK2	84	93
CDC2L1	85	93
RPS6KA5(Kin.Dom.2-C-terminal)	85	93
RIPK5	88	93
HASPIN	91	93
CDKL3	94	93
PKN1	97	93
BRAF(V600E)	100	93
HUNK	100	93
PIK3CA	100	93
SNARK	54	94
RSK1(Kin.Dom.1-N-terminal)	66	94
CSK	70	94
EGFR(S752-I759del)	83	94
CSNK1G1	86	94
FYN	90	94
FLT3(ITD)	93	94
TAK1	99	94
CLK4	100	94
FLT4	70	95
DAPK3	81	95
NEK5	84	95
CDK11	86	95
RIOK3	91	95

PYK2	95	95
MKNK2	99	95
p38-delta	99	95
CSNK1G2	100	95
CSNK2A1	100	95
JNK3	100	95
PKAC-beta	100	95
RSK1(Kin.Dom.2-C-terminal)	100	95
RSK4(Kin.Dom.1-N-terminal)	100	95
KIT(V559D,V654A)	61	96
RET(V804L)	74	96
PRKCI	82	96
RSK2(Kin.Dom.2-C-terminal)	85	96
PHKG2	89	96
CDK5	92	96
BRSK2	93	96
PRKD2	94	96
MAPKAPK5	95	96
NEK2	95	96
CDK9	97	96
TLK1	98	96
EPHA4	99	96
ACVR2B	100	96
ADCK3	100	96
PKN2	100	96
TAOK2	100	96
PAK6	73	97
CAMK1D	78	97
NEK4	83	97
FLT3(ITD,D835V)	91	97
NEK1	91	97
SIK	93	97
CAMK2B	94	97
SNRK	94	97
HIPK2	96	97
ADCK4	100	97
CAMK1G	100	97
INSRR	100	97
MUSK	100	97
TRKB	100	97
KIT(V559D)	68	98
TRPM6	71	98
EGFR(E746-A750del)	86	98
YES	87	98
CDC2L2	91	98
NEK11	91	98
ITK	93	98
LIMK1	93	98
MINK	95	98

PRKR	95	98
EPHB6	96	98
ARK5	100	98
DDR2	100	98
IKK-epsilon	100	98
MYLK4	100	98
STK39	100	98
YSK1	100	98
NEK7	72	99
DCAMKL2	83	99
DRAK1	88	99
EGFR(L747-T751del,Sins)	91	99
MEK1	93	99
PRKG2	93	99
EPHB4	94	99
CDK7	97	99
ERBB4	98	99
PRKCE	98	99
PLK3	99	99
FLT3(D835V)	100	99
PIK3CA(E545A)	100	99
PIM3	100	99
KIT(V559D,T670I)	71	100
CSF1R	74	100
FRK	74	100
FLT1	75	100
PRP4	80	100
DYRK1A	81	100
PFTAIRE2	81	100
PFTK1	82	100
ERK5	84	100
NEK6	85	100
MEK3	86	100
PIM1	86	100
TRKC	87	100
RIOK1	88	100
ABL1(F317I)-phosphorylated	89	100
ERBB2	89	100
HIPK3	89	100
PAK3	89	100
ASK1	90	100
MARK4	90	100
AURKB	91	100
CDK4-cyclinD1	91	100
MAP3K3	91	100
NLK	91	100
ALK	92	100
BTK	92	100
EGFR(L861Q)	92	100

FLT3	92	100
FAK	93	100
PIP5K1C	93	100
PIP5K2C	93	100
ROCK2	93	100
ULK3	93	100
IRAK4	94	100
RSK4(Kin.Dom.2-C-terminal)	94	100
ABL1(M351T)-phosphorylated	95	100
BRSK1	95	100
CAMK2G	95	100
ERK2	95	100
LTK	95	100
MEK2	95	100
RET	95	100
RPS6KA4(Kin.Dom.2-C-terminal)	95	100
AMPK-alpha2	96	100
EPHA8	96	100
GCN2(Kin.Dom.2,S808G)	96	100
KIT(D816H)	96	100
MEK4	96	100
RIPK1	96	100
SBK1	96	100
TNK2	96	100
ABL2	97	100
EGFR(G719S)	97	100
EPHA7	97	100
MAP4K4	97	100
SGK2	97	100
TLK2	97	100
ANKK1	98	100
CTK	98	100
FLT3(R834Q)	98	100
IRAK3	98	100
OSR1	98	100
STK33	98	100
CDKL5	99	100
DRAK2	99	100
ERK3	99	100
p38-alpha	99	100
AAK1	100	100
ABL1(E255K)-phosphorylated	100	100
ABL1(F317L)-phosphorylated	100	100
ABL1(H396P)-phosphorylated	100	100
ABL1(Q252H)-phosphorylated	100	100
ABL1(T315I)-phosphorylated	100	100
ABL1(Y253F)-phosphorylated	100	100
ACVR2A	100	100
AKT1	100	100

ALK(C1156Y)	100	100
ALK(L1196M)	100	100
AMPK-alpha1	100	100
AURKA	100	100
AURKC	100	100
BMPR2	100	100
BMX	100	100
CAMK2D	100	100
CAMK4	100	100
CAMKK1	100	100
CAMKK2	100	100
CDC2L5	100	100
CDK3	100	100
CDK4	100	100
CDK4-cyclinD3	100	100
CHEK2	100	100
CLK1	100	100
CLK3	100	100
CSNK1E	100	100
CSNK1G3	100	100
DAPK1	100	100
DCAMKL1	100	100
DCAMKL3	100	100
DMPK	100	100
DMPK2	100	100
DYRK2	100	100
EGFR	100	100
EGFR(G719C)	100	100
EGFR(L747-E749del, A750P)	100	100
EGFR(L747-S752del, P753S)	100	100
EGFR(L858R)	100	100
EGFR(L858R,T790M)	100	100
EPHA2	100	100
EPHA3	100	100
EPHB2	100	100
ERK1	100	100
ERK8	100	100
ERN1	100	100
FER	100	100
FGFR2	100	100
FGFR3	100	100
FGFR4	100	100
FLT3(ITD,F691L)	100	100
FLT3-autoinhibited	100	100
GRK1	100	100
GRK2	100	100
GRK3	100	100
GSK3B	100	100
HCK	100	100

IGF1R	100	100
IKK-alpha	100	100
IKK-beta	100	100
IRAK1	100	100
JAK1(JH2domain-pseudokinase)	100	100
JAK2(JH1domain-catalytic)	100	100
KIT(A829P)	100	100
KIT(D816V)	100	100
KIT-autoinhibited	100	100
LATS1	100	100
LCK	100	100
LIMK2	100	100
LKB1	100	100
LOK	100	100
LRRK2	100	100
LYN	100	100
MAP3K15	100	100
MAP4K2	100	100
MAP4K3	100	100
MAPKAPK2	100	100
MET	100	100
MET(Y1235D)	100	100
MKNK1	100	100
MLK1	100	100
MLK3	100	100
MRCKA	100	100
MRCKB	100	100
MST1	100	100
MST3	100	100
MST4	100	100
MYLK	100	100
MYO3A	100	100
MYO3B	100	100
NEK10	100	100
NIK	100	100
PAK1	100	100
PAK7	100	100
PCTK1	100	100
PDGFRA	100	100
PDPK1	100	100
PFCDPK1(P.falciparum)	100	100
PFPK5(P.falciparum)	100	100
PHKG1	100	100
PIK3CA(C420R)	100	100
PIK3CA(H1047L)	100	100
PIK3CA(H1047Y)	100	100
PIK3CA(M1043I)	100	100
PIM2	100	100
PIP5K1A	100	100

PIP5K2B	100	100
PKAC-alpha	100	100
PKMYT1	100	100
PLK2	100	100
PLK4	100	100
PRKD1	100	100
PRKX	100	100
QSK	100	100
RIPK2	100	100
RPS6KA5(Kin.Dom.1-N-terminal)	100	100
RSK2(Kin.Dom.1-N-terminal)	100	100
RSK3(Kin.Dom.2-C-terminal)	100	100
S6K1	100	100
SgK110	100	100
SGK3	100	100
SIK2	100	100
SLK	100	100
SRC	100	100
SRMS	100	100
SRPK3	100	100
STK35	100	100
STK36	100	100
SYK	100	100
TAOK1	100	100
TAOK3	100	100
TEC	100	100
TGFBR2	100	100
TIE1	100	100
TNIK	100	100
TNNI3K	100	100
TSSK1B	100	100
TYK2(JH1domain-catalytic)	100	100
TYK2(JH2domain-pseudokinase)	100	100
ULK2	100	100
VEGFR2	100	100
WEE1	100	100
YANK2	100	100
YSK4	100	100
ZAP70	100	100

	BAY 1895344 Kd [nM]	BAY 1895344 <50% Ctrl @ 100 nM	BAY 1895344 <50% Ctrl @ 1000 nM
DYRK1B	25000	28	11
mTOR	24	41	2.2
GAK	580	-	27
GSK3A	>30000	-	31
RIOK2	660	-	24
VPS34	3200	46	17

Figure S1. Determination of K_D values at DiscoverX for identified off-target kinases (< 50% of control at 100 nM or 1000 nM compound concentration).

LC-MS Methods for Determination of Purity

Method 1

Instrument: Waters Acquity UPLCMS SingleQuad; Column: Acquity UPLC BEH C18 1.7 µm, 50x2.1mm; eluent A: water + 0.1 vol % formic acid (99%), eluent B: acetonitrile; gradient: 0-1.6 min 1-99% B, 1.6-2.0 min 99% B; flow 0.8 ml/min; temperature: 60 °C; DAD scan: 210-400 nm.

Method 2

Instrument: Waters Acquity UPLCMS SingleQuad; Column: Acquity UPLC BEH C18 1.7 µm, 50x2.1mm; eluent A: water + 0.2 vol % NH_3 (32%), eluent B: acetonitrile; gradient: 0-1.6 min 1-99% B, 1.6-2.0 min 99% B; flow 0.8 ml/min; temperature: 60 °C; DAD scan: 210-400 nm.

Method 3

Instrument: Agilent; Column: Ascentis Express C18, 2.7 µm, 3 cm x 2.1 mm; eluent A: water + 0.1 vol % formic acid (99%), eluent B: methanol + 0.1% formic acid (99%); temperature: 30 °C; DAD scan: 210-400 nm; gradient and flow rate:

time in min	%A	%B	flow rate in ml/min
1.0	95	5	0.8
4.0	0	100	0.8
5.0	0	100	0.8
6.0	95	5	0.8
6.5	95	5	0.8

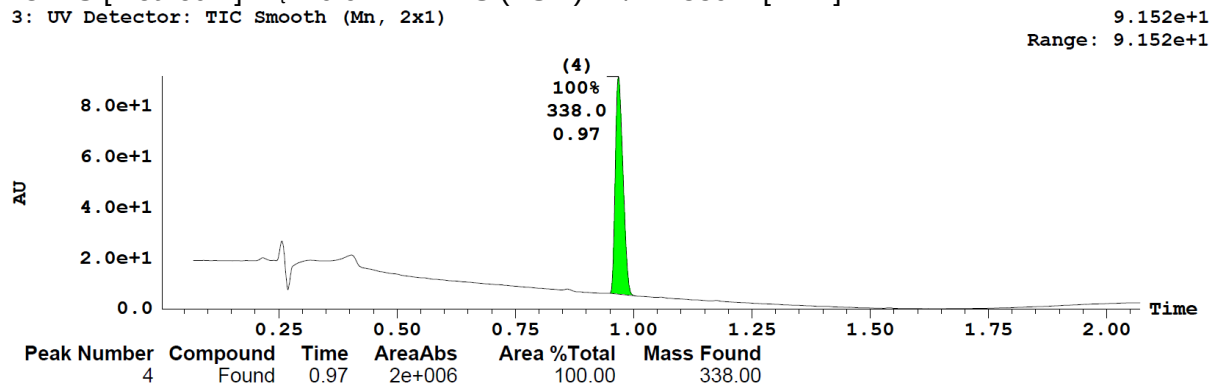
Method 4

Instrument MS: Waters TOF instrument; UPLC System: Waters Acquity I-CLASS; Column: Waters Acquity UPLC HSS T3 1.8 µm 50 x 1 mm; eluent A: 1 L water + 0.100 mL formic acid (99%), eluent B: 1 l acetonitrile + 0.100 ml formic acid (99%); gradient: 0.0 min 92.5% A →0.2 min 92.5% A → 0.6 min 10% A → 1.3 min 5% A Oven: 50°C; Flow: 0.45 ml/min; UV-Detection: 210 - 300 nm.

Original Data

Example 2

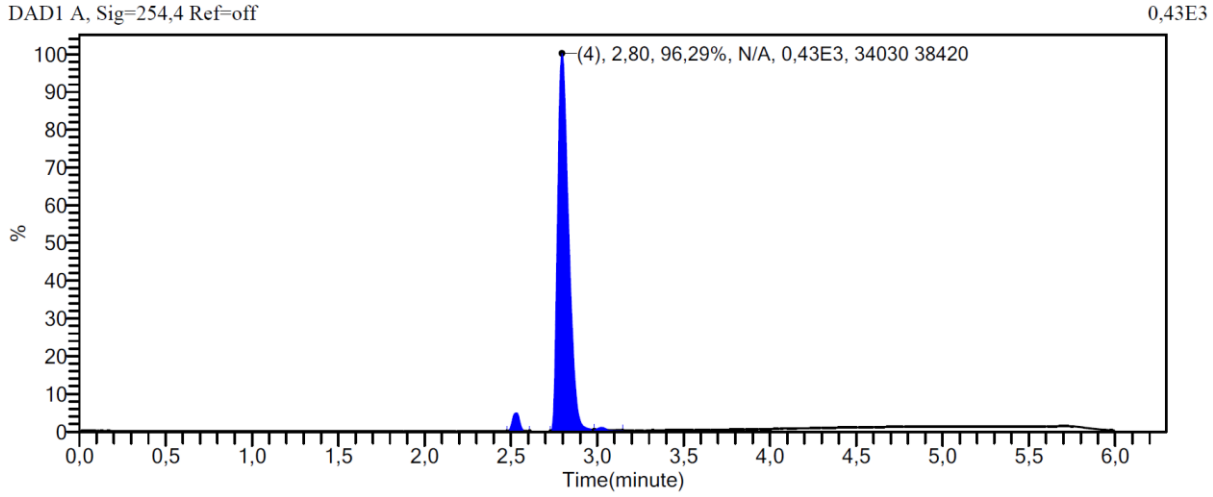
LC-MS [Method 1]: R_t = 0.97 min. MS (ESI+): *m/z* = 339.2 $[M+H]^+$.

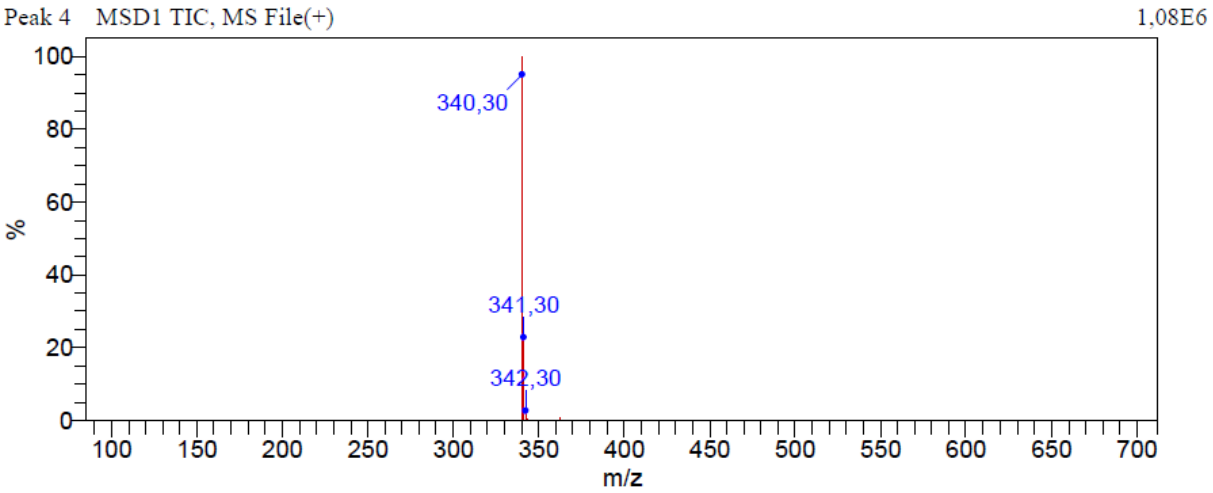


Peak Number	Compound	Time	AreaAbs	Area %Total	Mass Found
4	Found	0.97	2e+006	100.00	338.00

Example 3

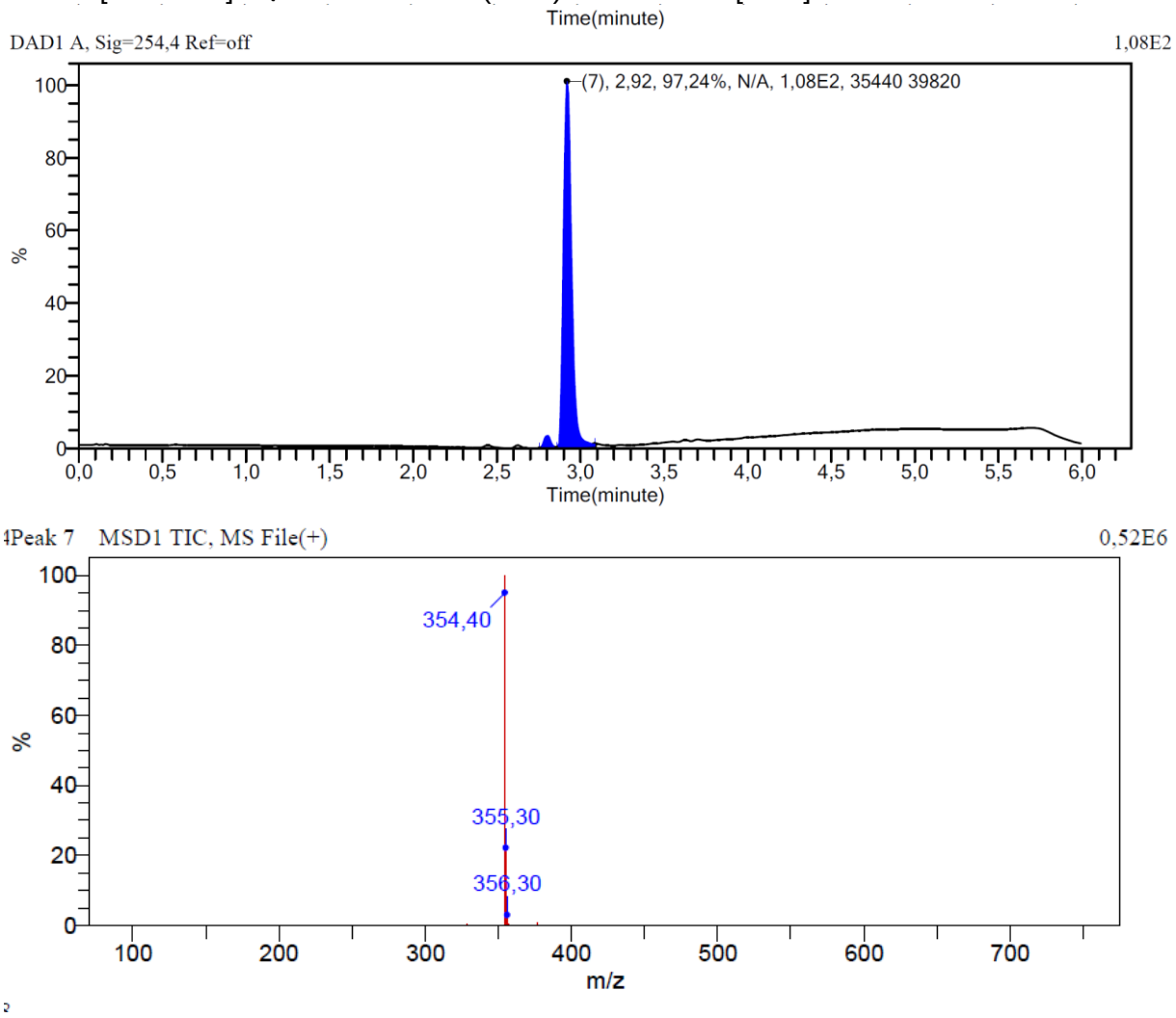
LC-MS [Method 3]: R_t = 2.80 min. MS (ESI+): m/z = 340.3 $[M+H]^+$.





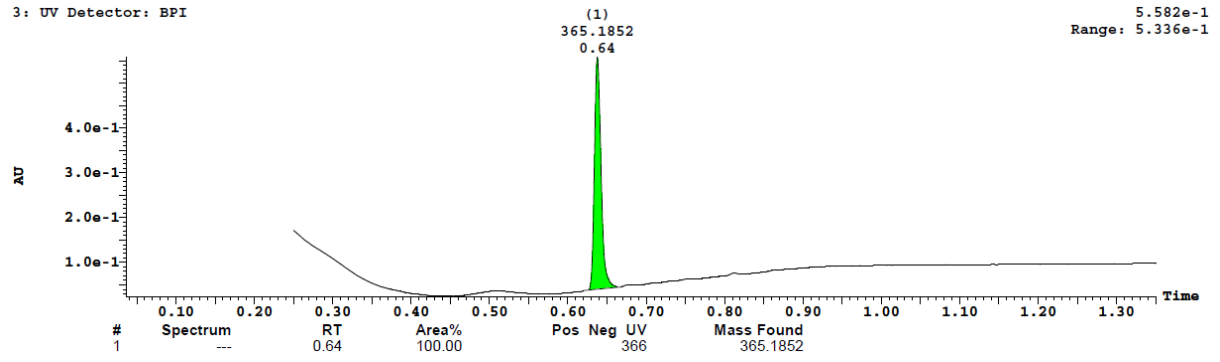
Example 4

LC-MS [Method 3]: R_t = 2.92 min. MS (ESI+): *m/z* = 354.4 $[M+H]^+$.



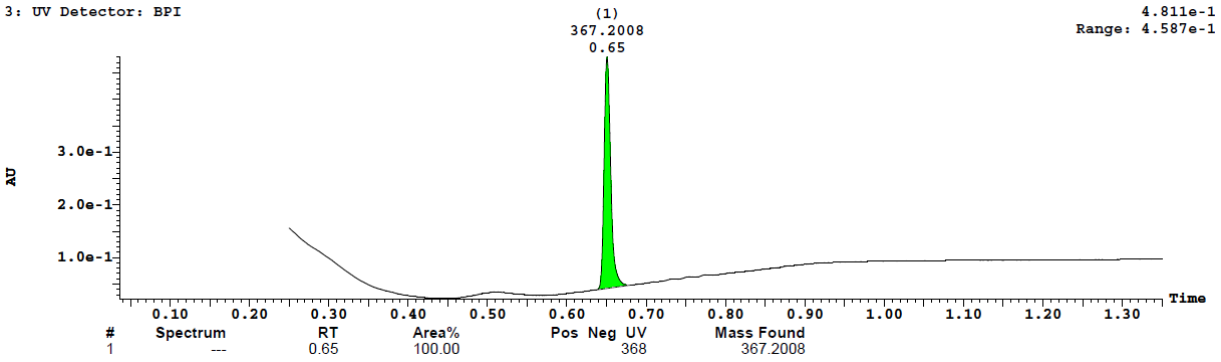
Example 5

LC-MS [Method 4]: R_t = 0.64 min. MS (ESI+): *m/z* = 366.2 $[M+H]^+$.



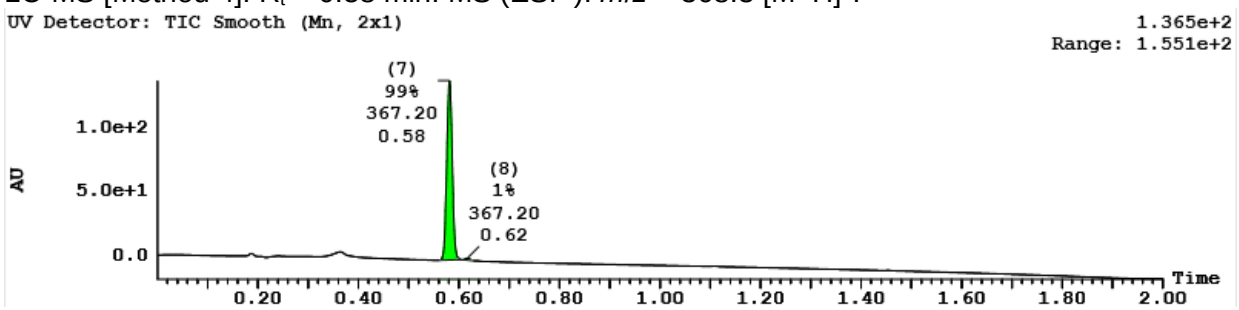
Example 6

LC-MS [Method 4]: R_t = 0.65 min. MS (ESI+): *m/z* = 368.3 $[M+H]^+$.



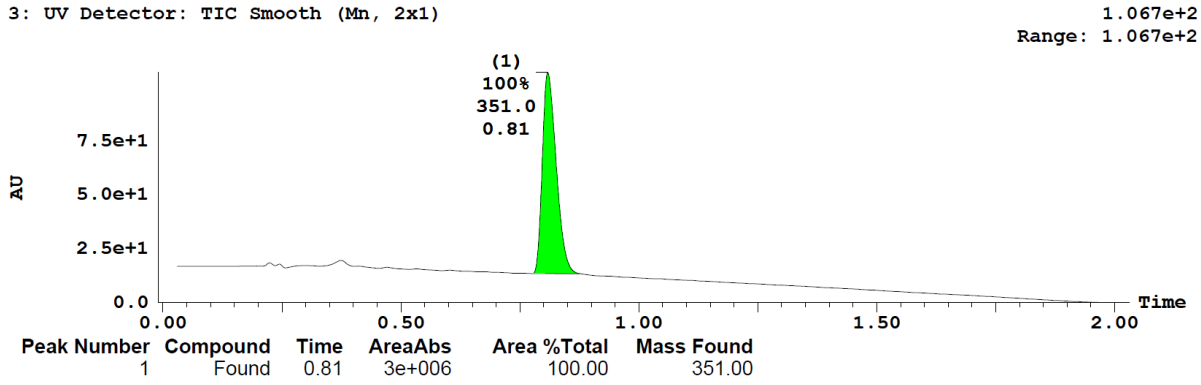
Example 7

LC-MS [Method 4]: R_t = 0.58 min. MS (ESI+): *m/z* = 368.3 $[M+H]^+$.



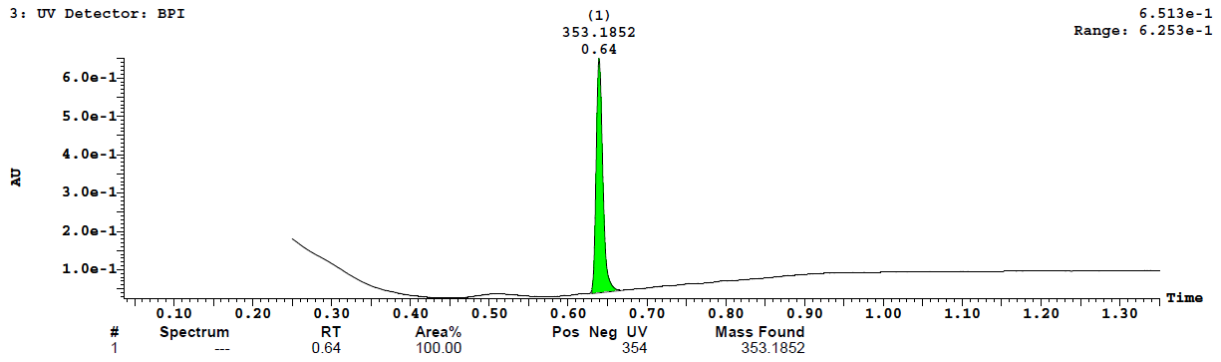
Example 8

LC-MS [Method 1]: R_t = 0.81 min. MS (ESI+): *m/z* = 352.3 $[M+H]^+$.



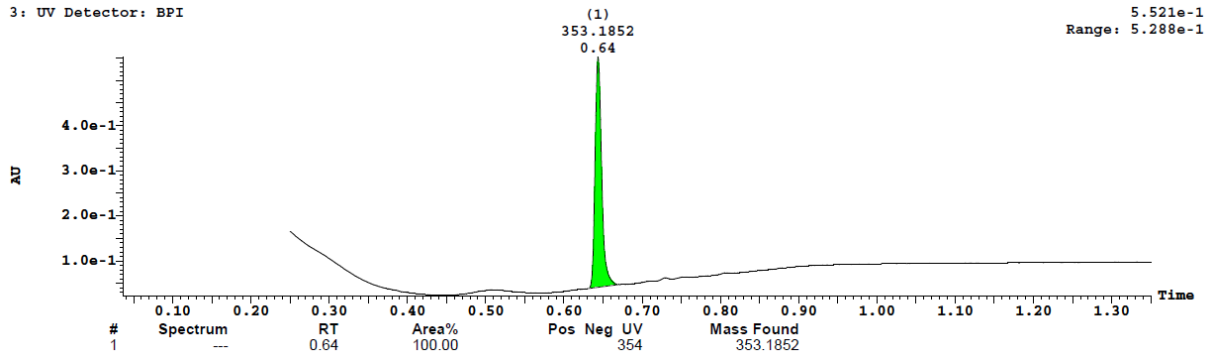
Example 9

LC-MS [Method 4]: R_t = 0.64 min. MS (ESI+): *m/z* = 354.2 $[M+H]^+$.



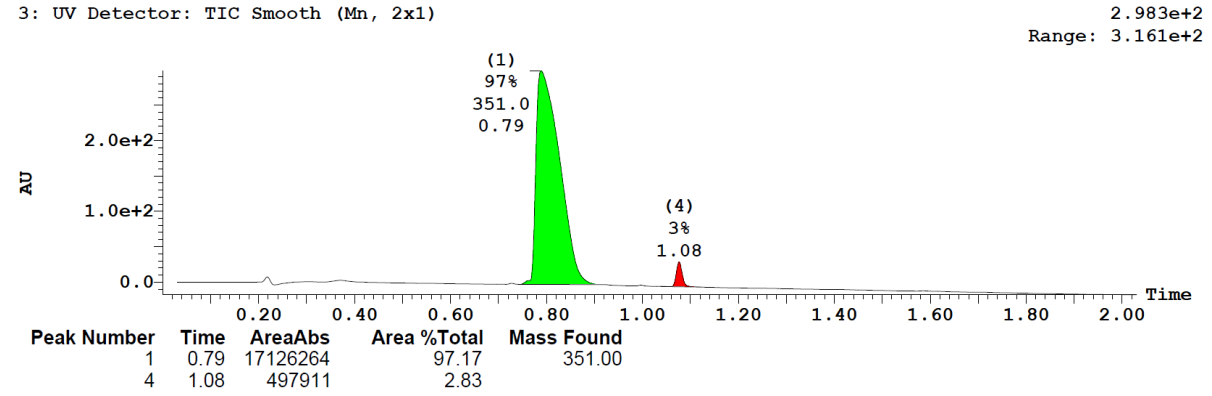
Example 10

LC-MS [Method 4]: R_t = 0.64 min. MS (ESI+): *m/z* = 354.2 $[M+H]^+$.



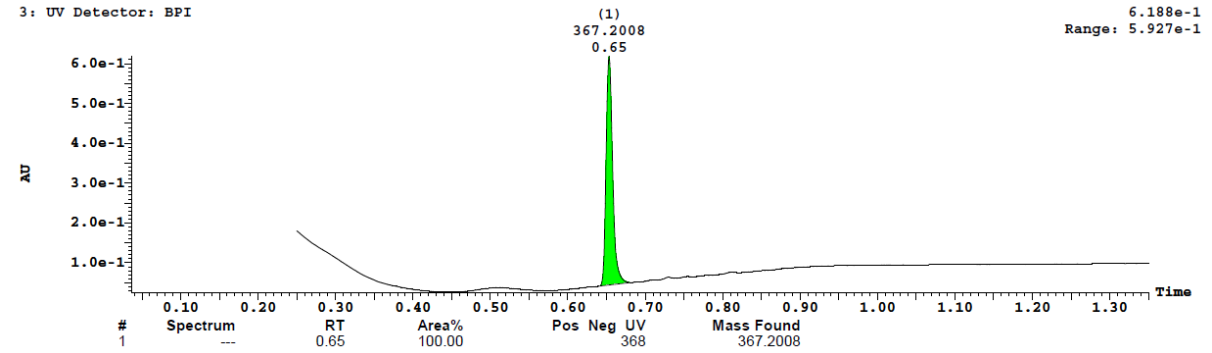
Example 11

LC-MS [Method 1]: R_t = 0.79 min. MS (ESI+): *m/z* = 352.0 $[M+H]^+$.



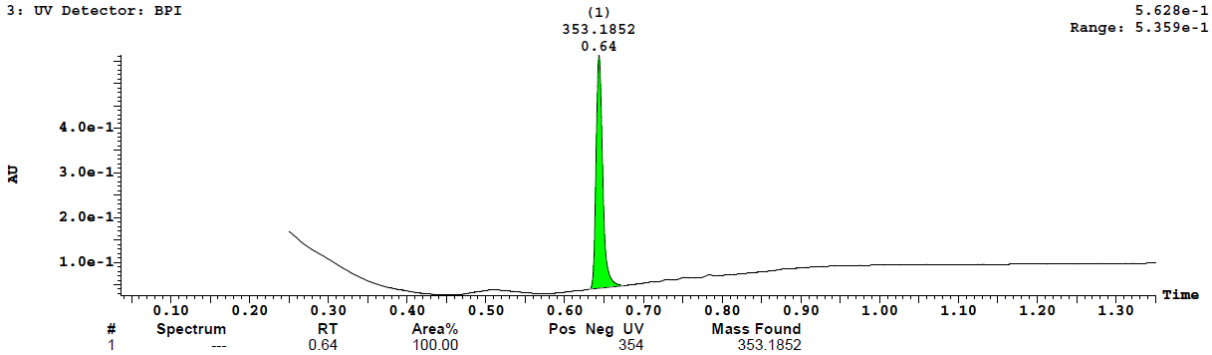
Example 12

LC-MS [Method 4]: R_t = 0.65 min. MS (ESI+): *m/z* = 368.2 $[M+H]^+$.



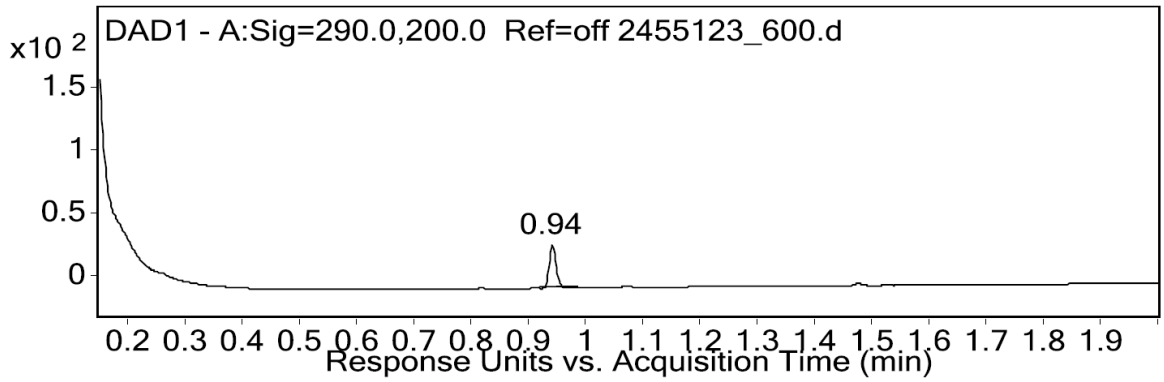
Example 13

LC-MS [Method 4]: R_t = 0.64 min. MS (ESI+): *m/z* = 354.2 $[M+H]^+$.



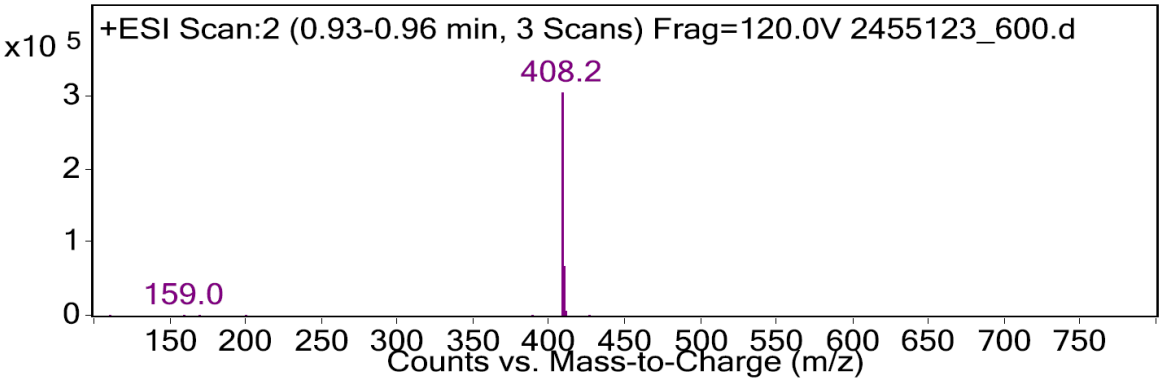
Example 14

LC-MS [Method 3]: R_t = 0.94 min. MS (ESI+): *m/z* = 408.2 $[M+H]^+$.



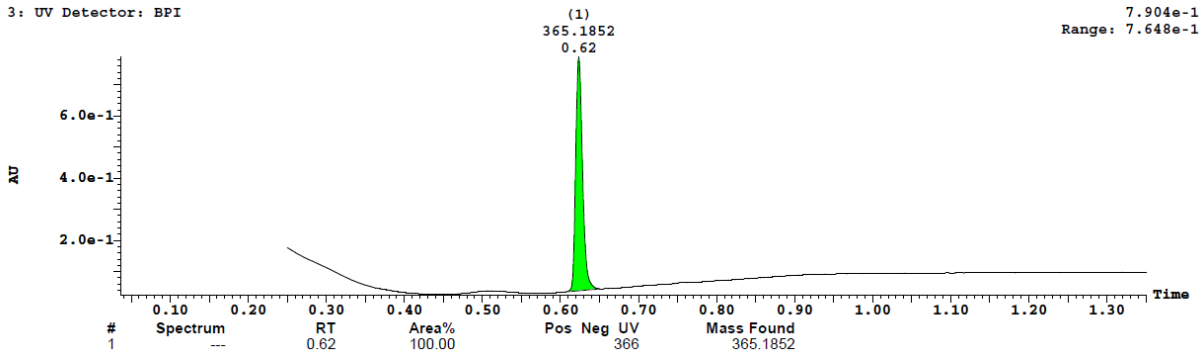
Integration Peak List

Peak	RT	Height	Area	AreaSumPercent
1	0.94	34.01	28.76	100



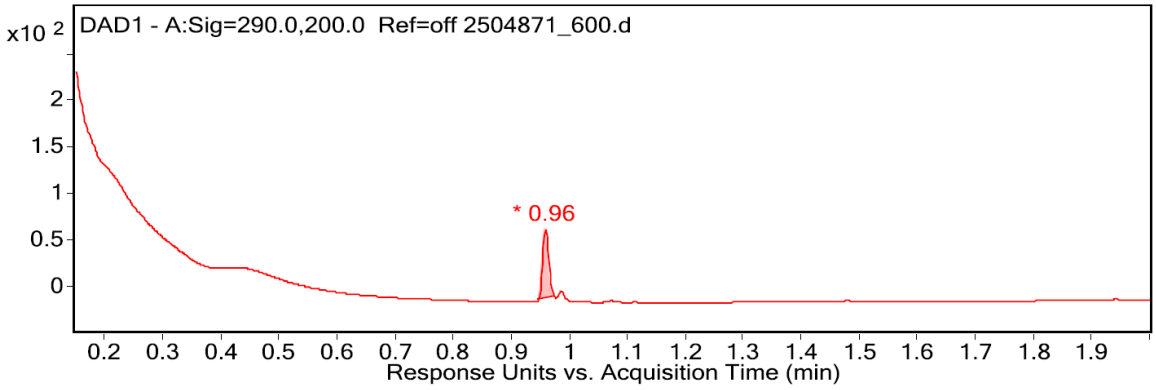
Example 15

LC-MS [Method 4]: R_t = 0.62 min. MS (ESI+): *m/z* = 366.2 $[M+H]^+$.



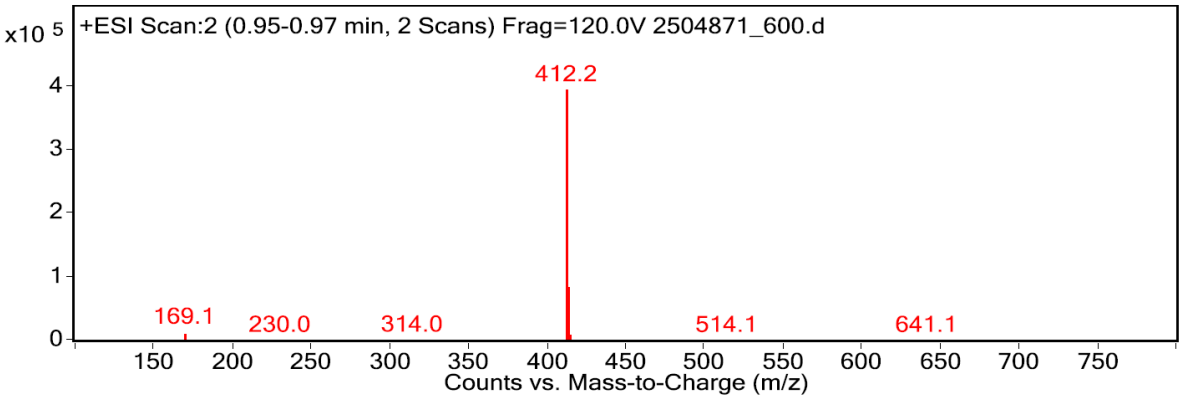
Example 16

LC-MS [Method 3]: R_t = 0.96 min. MS (ESI+): *m/z* = 412.2 $[M+H]^+$.



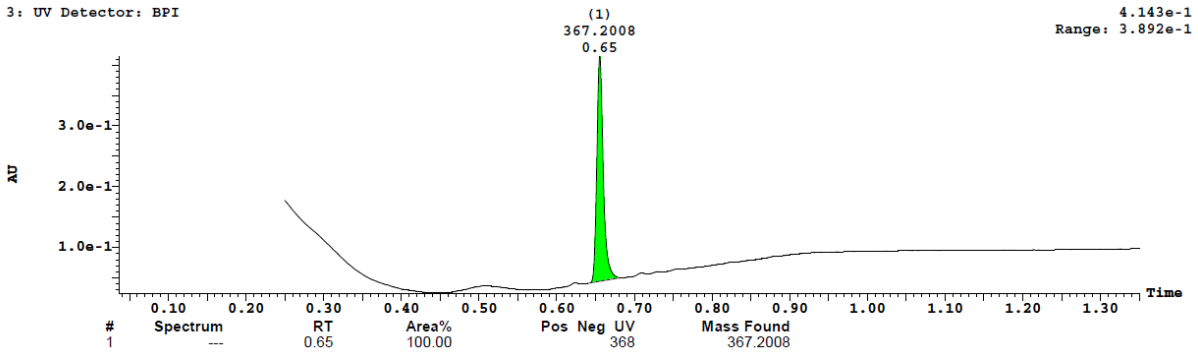
Integration Peak List

Peak	RT	Height	Area	AreaSumPercent
1	0.96	75.1	56.78	100



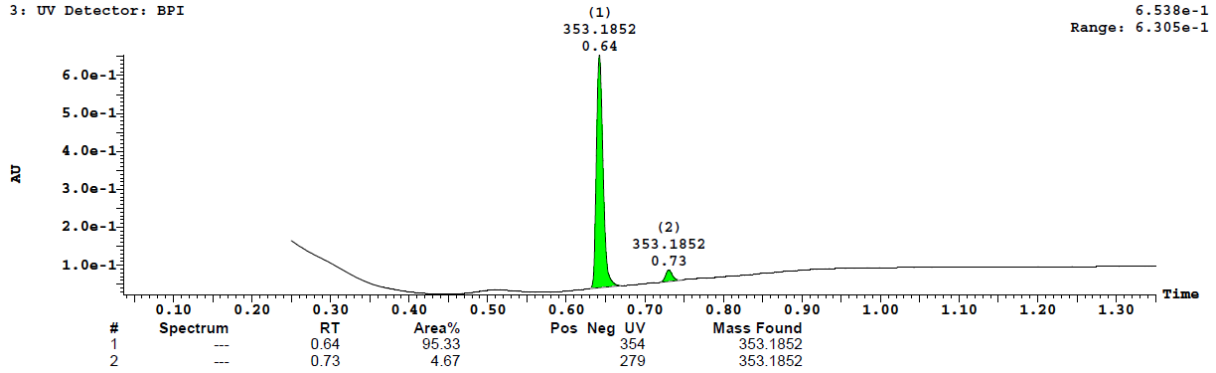
Example 17

LC-MS [Method 4]: R_t = 0.65 min. MS (ESI+): *m/z* = 368.2 $[M+H]^+$.



Example 18

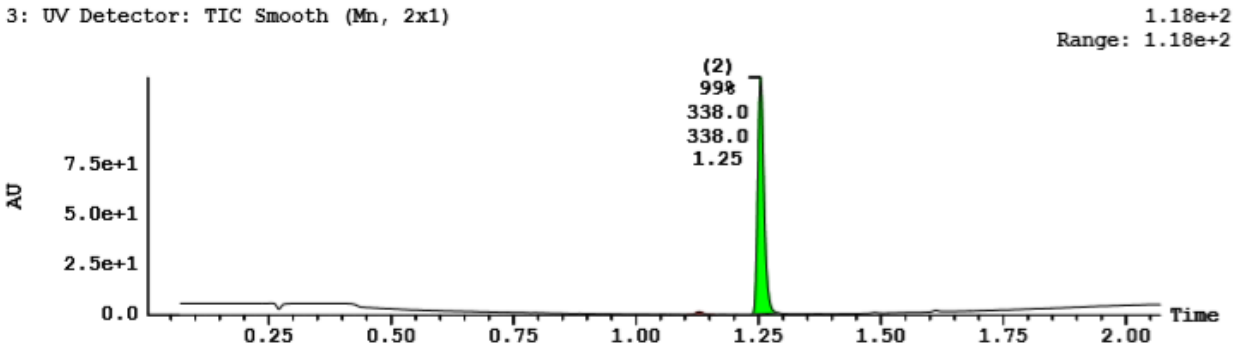
LC-MS [Method 4]: R_t = 0.64 min. MS (ESI+): *m/z* = 354.2 $[M+H]^+$.



#	Spectrum	RT	Area%	Pos Neg UV	Mass Found
1	---	0.64	95.33	354	353.1852
2	---	0.73	4.67	279	353.1852

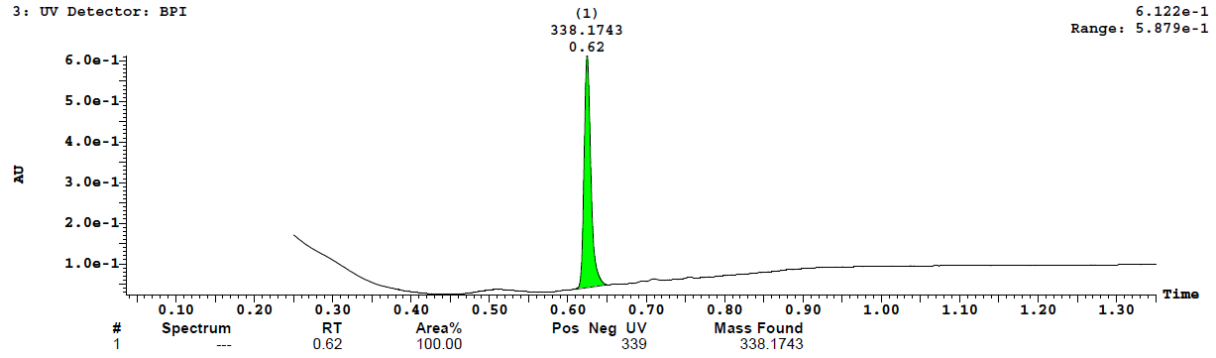
Example 19

LC-MS [Method 2]: R_t = 1.25 min. MS (ESI+): *m/z* = 339.2 $[M+H]^+$.



Example 20

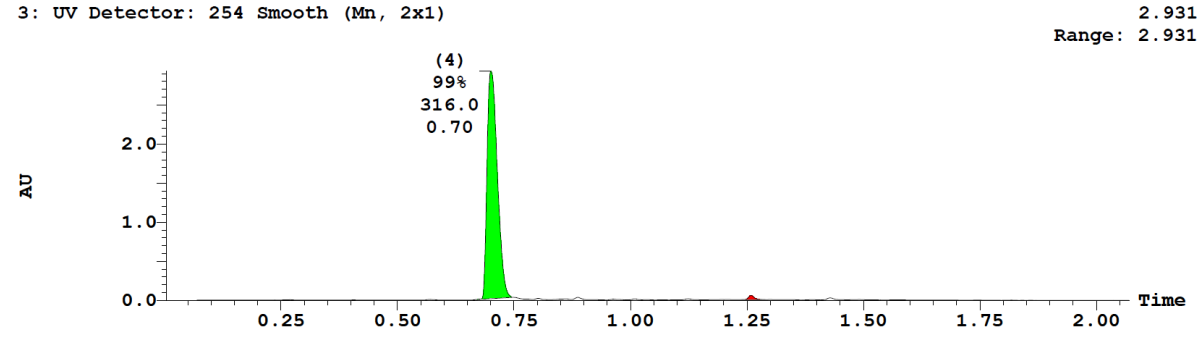
LC-MS [Method 4]: R_t = 0.62 min. MS (ESI+): *m/z* = 339.2 $[M+H]^+$.



#	Spectrum	RT	Area%	Pos Neg UV	Mass Found
1	---	0.62	100.00	339	338.1743

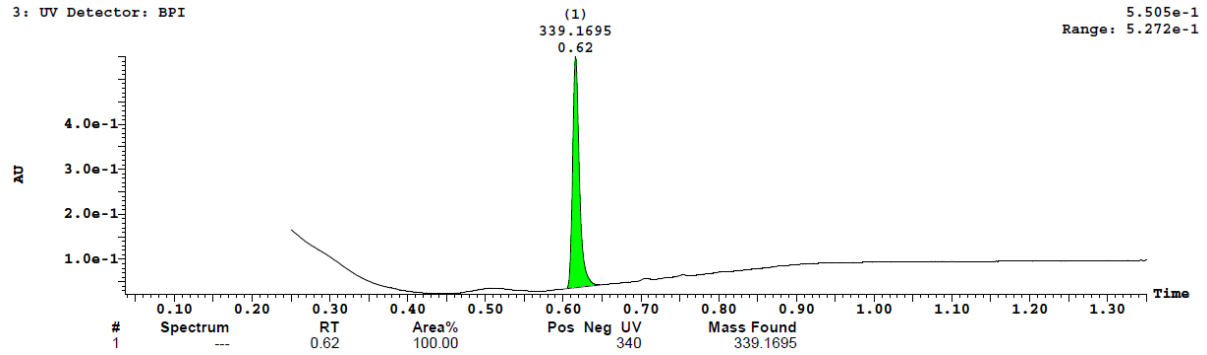
Example 21

LC-MS [Method 1]: R_t = 0.70 min. MS (ESI+): m/z = 317.0 $[M+H]^+$.



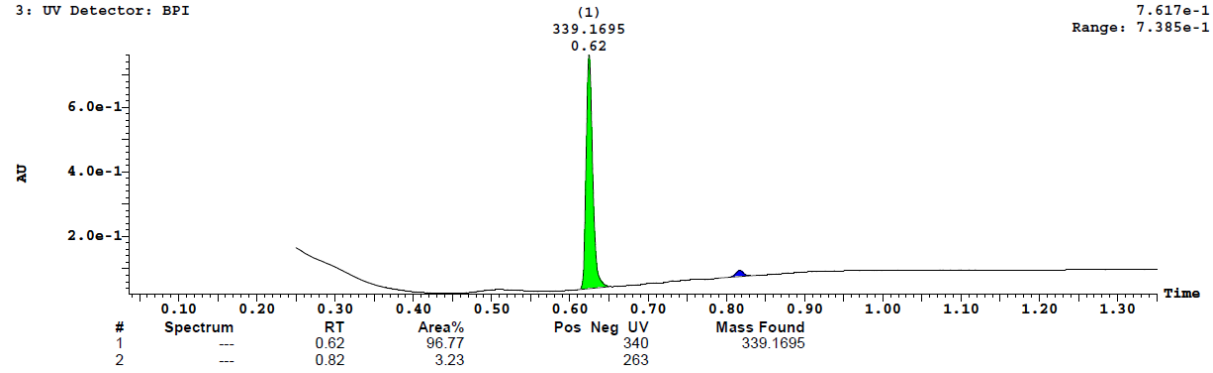
Example 22

LC-MS [Method 4]: R_t = 0.62 min. MS (ESI+): m/z = 340.2 $[M+H]^+$.



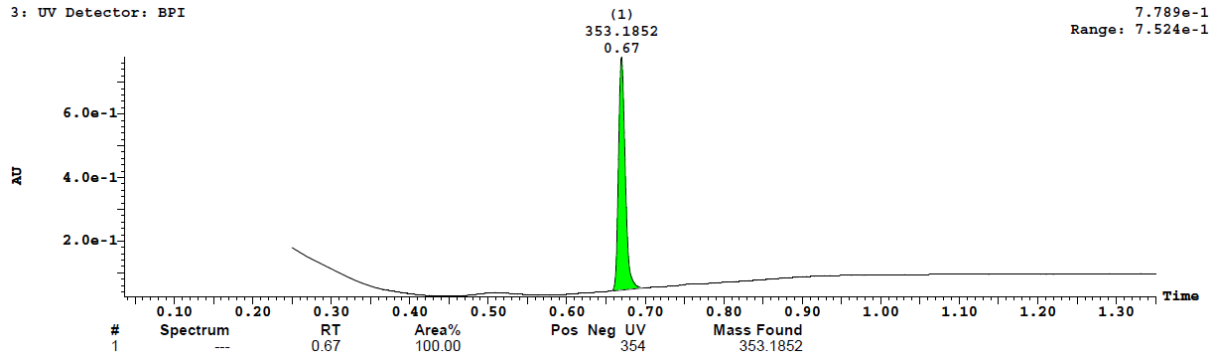
Example 23

LC-MS [Method 4]: R_t = 0.62 min. MS (ESI+): m/z = 340.3 $[M+H]^+$.



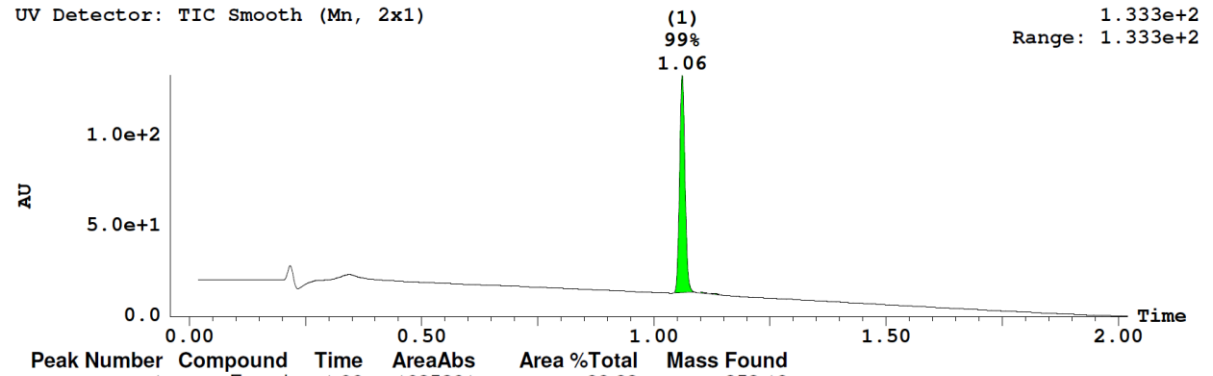
Example 24

LC-MS [Method 4]: R_t = 0.67 min. MS (ESI+): m/z = 354.3 $[M+H]^+$.



Example 25

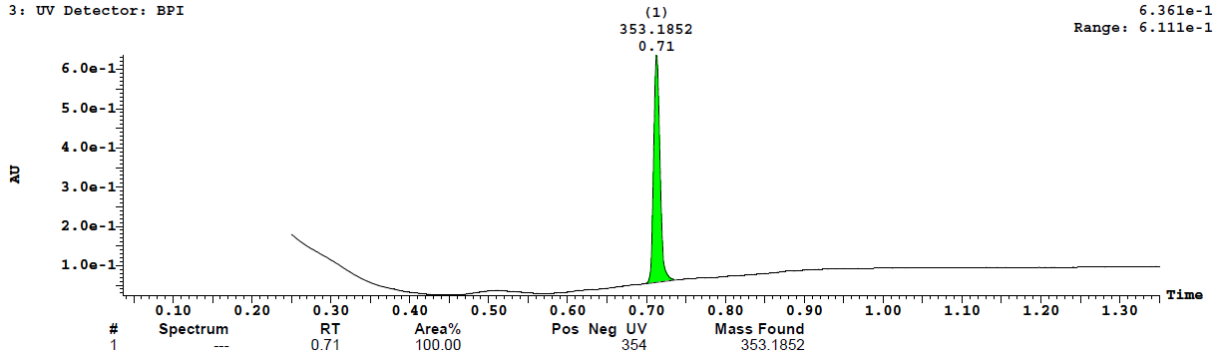
LC-MS [Method 1]: R_t = 1.06 min. MS (ESI+): m/z = 354.3 $[M+H]^+$.



Peak Number	Compound	Time	AreaAbs	Area %Total	Mass Found
1	Found	1.06	1635261	98.83	353.19
1	Found	1.10	7596	0.46	353.19
2	Found	1.13	11717	0.71	353.19

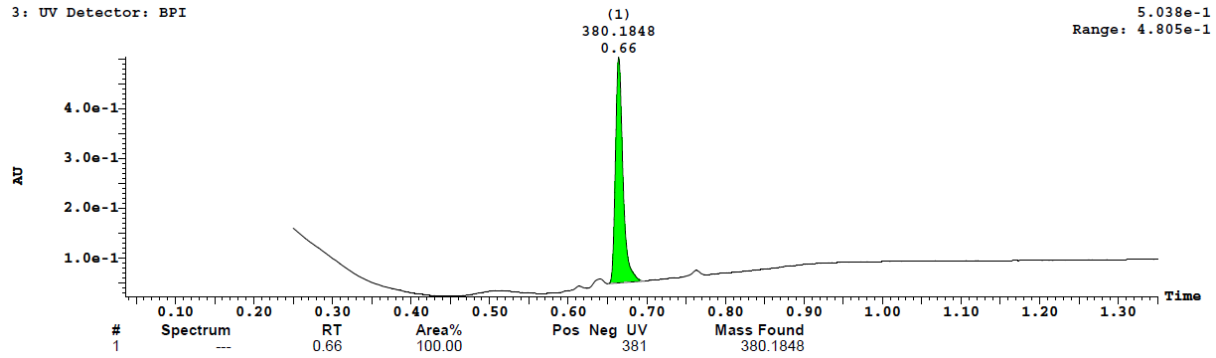
Example 26

LC-MS [Method 4]: R_t = 0.71 min. MS (ESI+): *m/z* = 354.3 $[M+H]^+$.



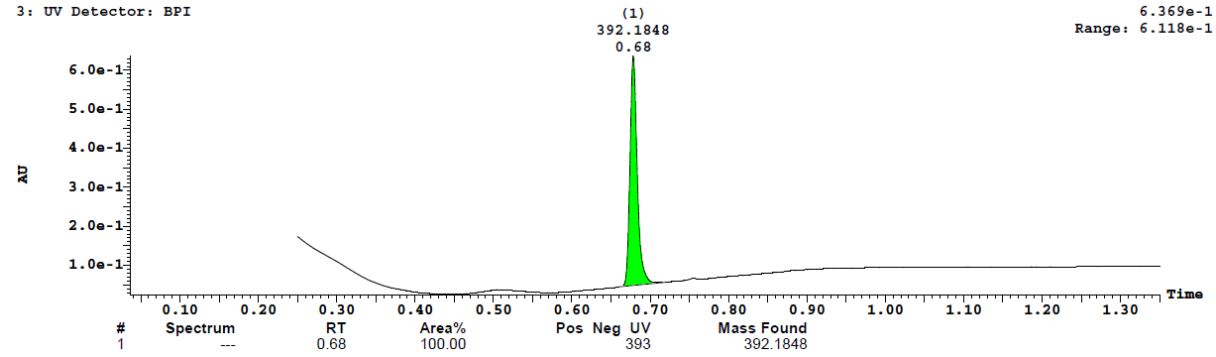
Example 27

LC-MS [Method 4]: R_t = 0.66 min. MS (ESI+): *m/z* = 381.2 $[M+H]^+$.



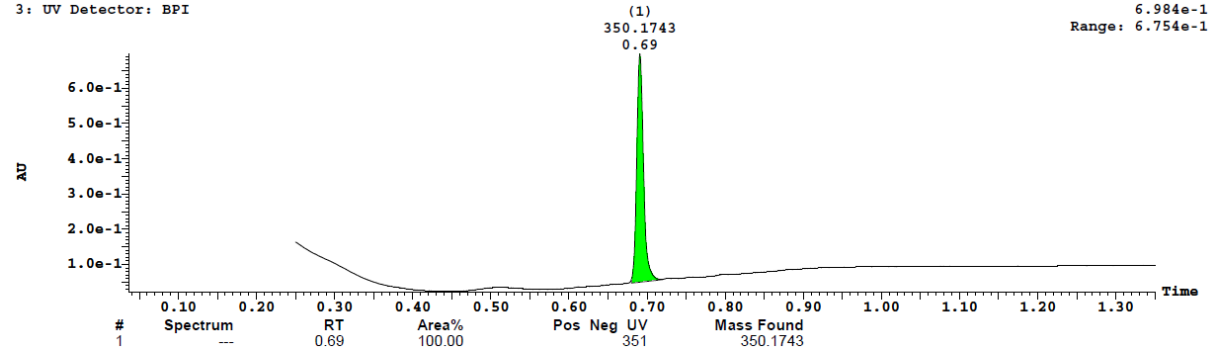
Example 28

LC-MS [Method 4]: R_t = 0.68 min. MS (ESI+): m/z = 393.3 $[M+H]^+$.



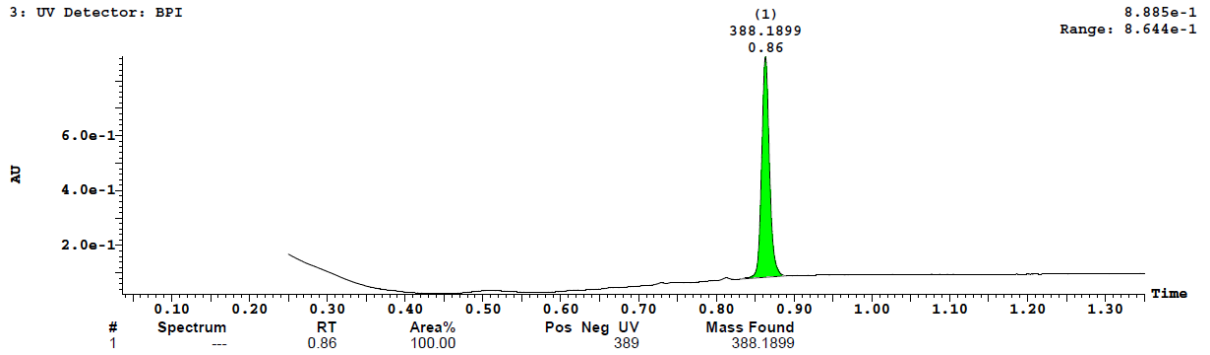
Example 29

LC-MS [Method 4]: R_t = 0.69 min. MS (ESI+): *m/z* = 351.2 $[M+H]^+$.



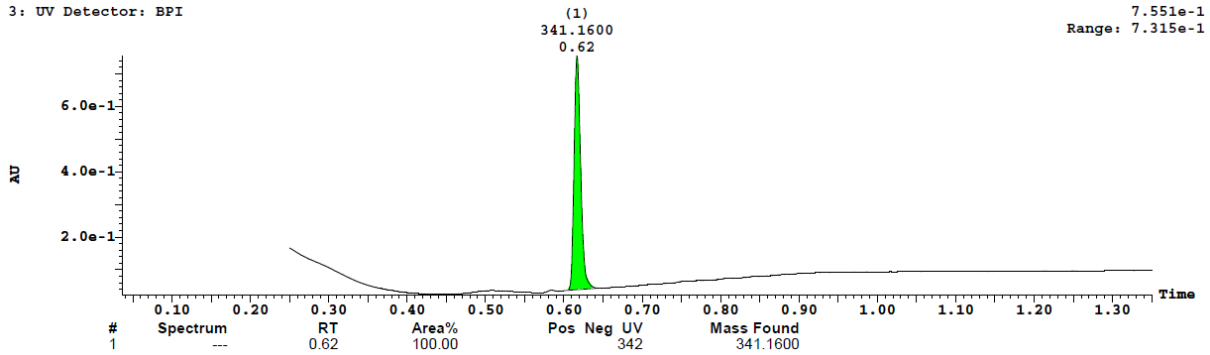
Example 30

LC-MS [Method 4]: R_t = 0.86 min. MS (ESI+): *m/z* = 389.3 $[M+H]^+$.



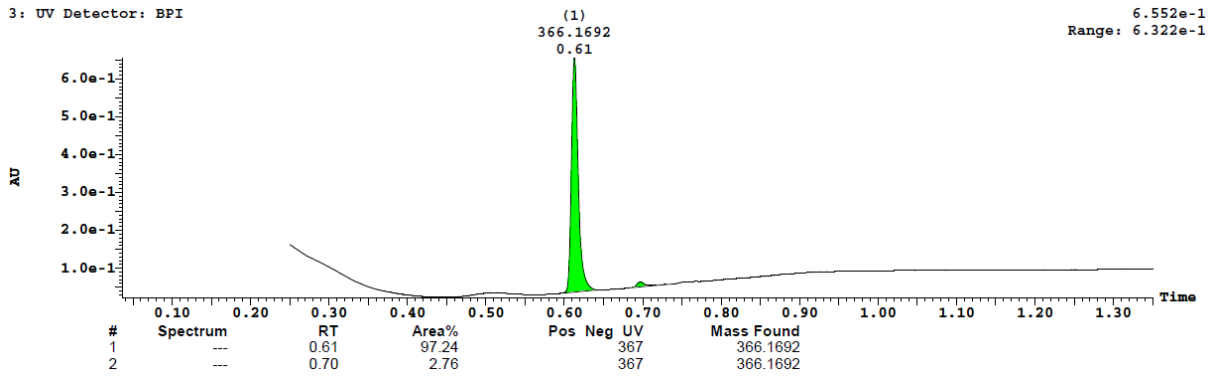
Example 31

LC-MS [Method 4]: R_t = 0.62 min. MS (ESI+): *m/z* = 342.2 $[M+H]^+$.



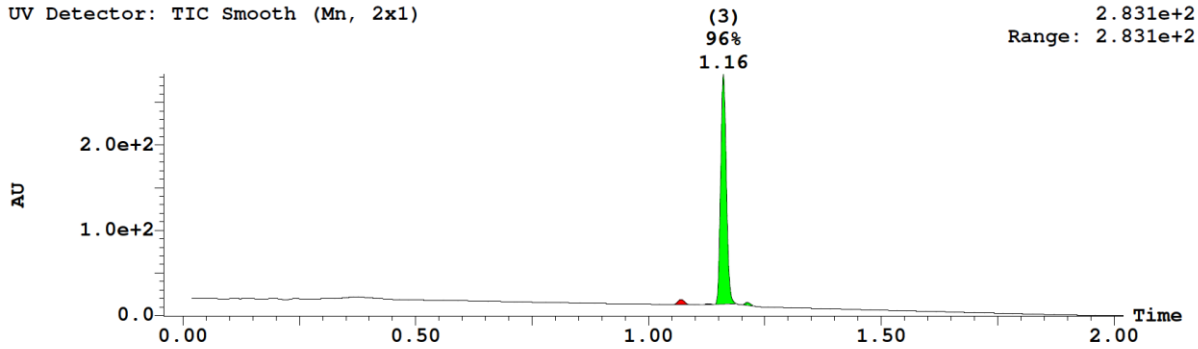
Example 32

LC-MS [Method 4]: R_t = 0.61 min. MS (ESI+): *m/z* = 367.0 $[M+H]^+$.



Example 33

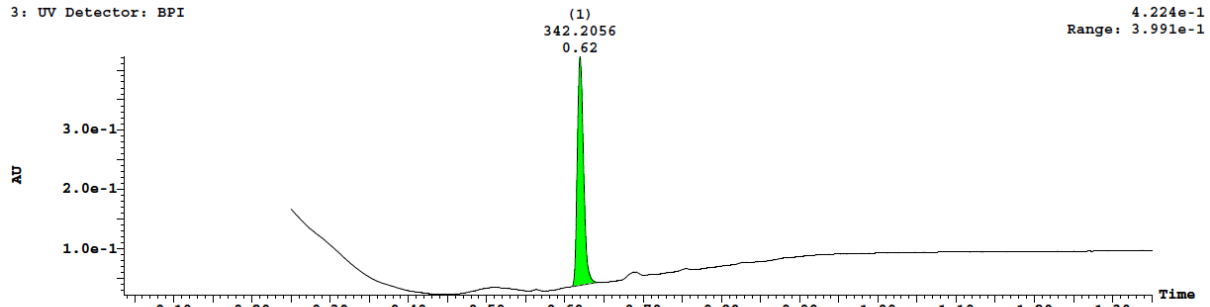
LC-MS [Method 1]: R_t = 1.16 min. MS (ESI+): *m/z* = 367.3 $[M+H]^+$.



Peak Number	Compound	Time	AreaAbs	Area %Total	Mass Found
1		1.07	95178	2.37	
2		1.13	15602	0.39	
3	Found	1.16	3853273	95.96	366.17
4	Found	1.21	51579	1.28	366.17

Example 34

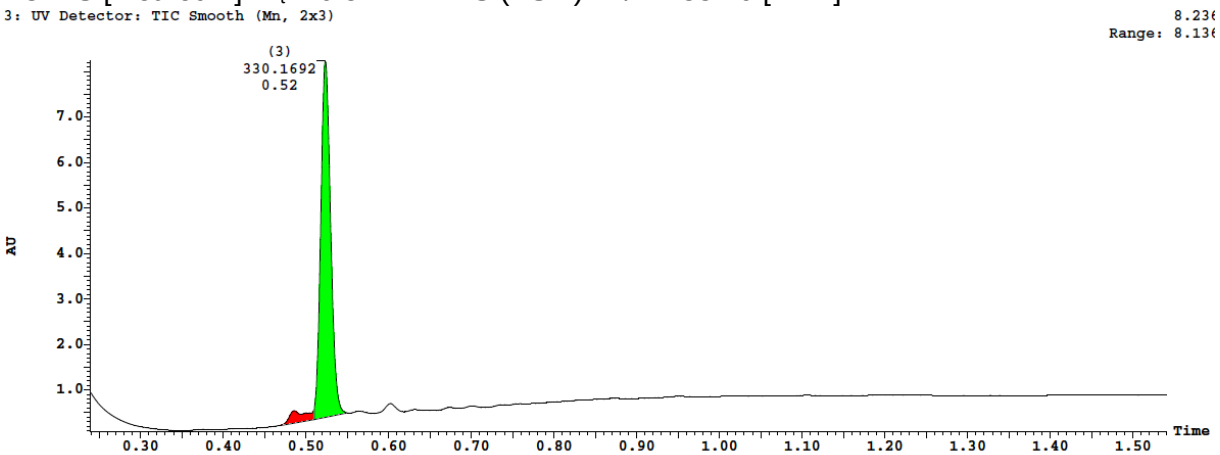
LC-MS [Method 4]: R_t = 0.62 min. MS (ESI+): *m/z* = 343.3 $[M+H]^+$.



#	Spectrum	RT	Area%	Pos	Neg	UV	Mass Found
1	---	0.62	100.00			343	342.2056

Example 35

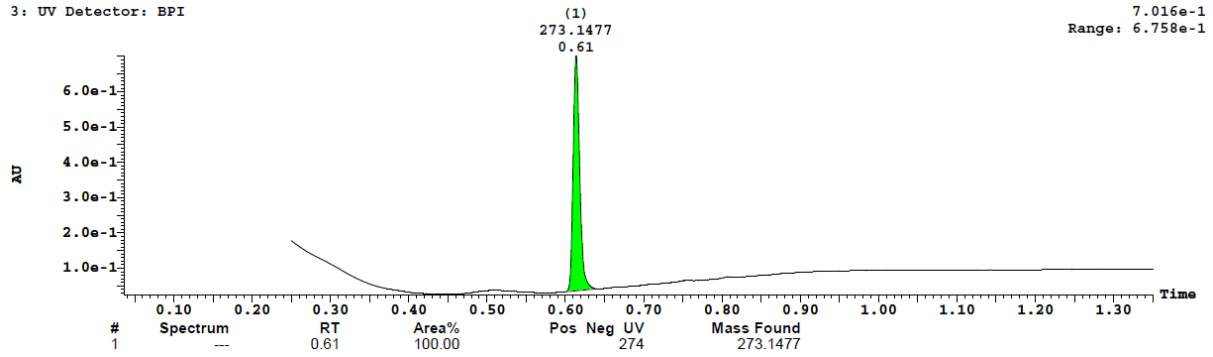
LC-MS [Method 1]: R_t = 0.52 min. MS (ESI+): *m/z* = 331.0 $[M+H]^+$.



Peak Number	Time	Area %Total	Mass Found	AreaAbs
2	0.49	4.84		5539
3	0.52	95.16	330.1692	108879

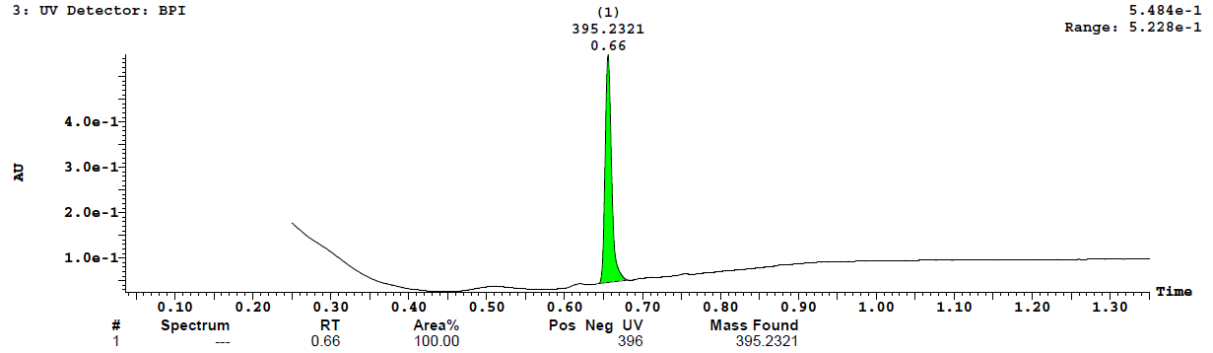
Example 36

LC-MS [Method 4]: R_t = 0.61 min. MS (ESI+): *m/z* = 274.2 $[M+H]^+$.



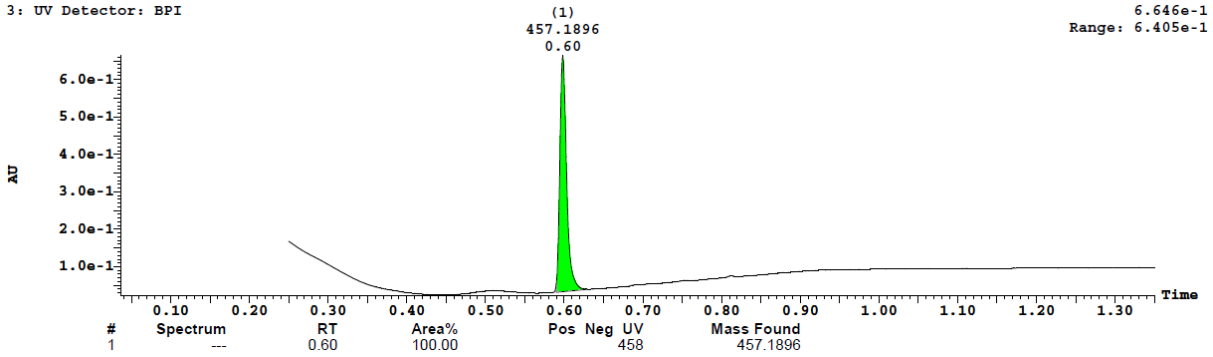
Example 37

LC-MS [Method 4]: R_t = 0.66 min. MS (ESI+): *m/z* = 396.3 $[M+H]^+$.



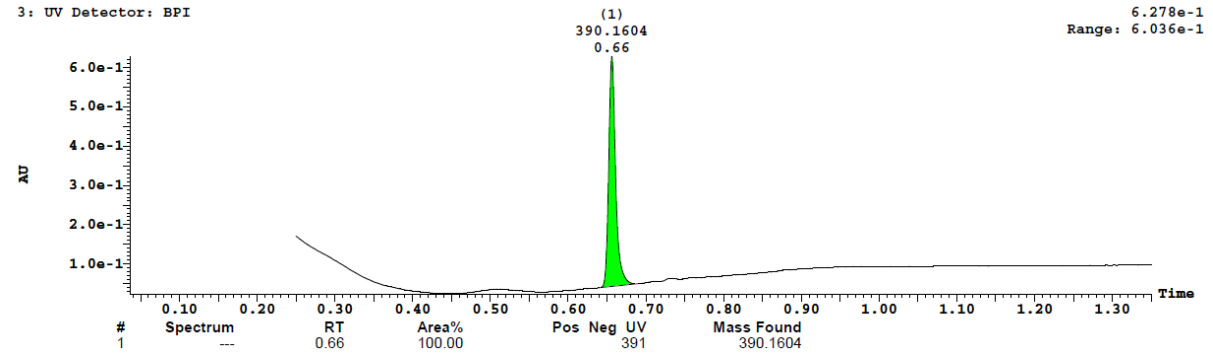
Example 38

LC-MS [Method 4]: R_t = 0.60 min. MS (ESI+): *m/z* = 458.3 $[M+H]^+$.



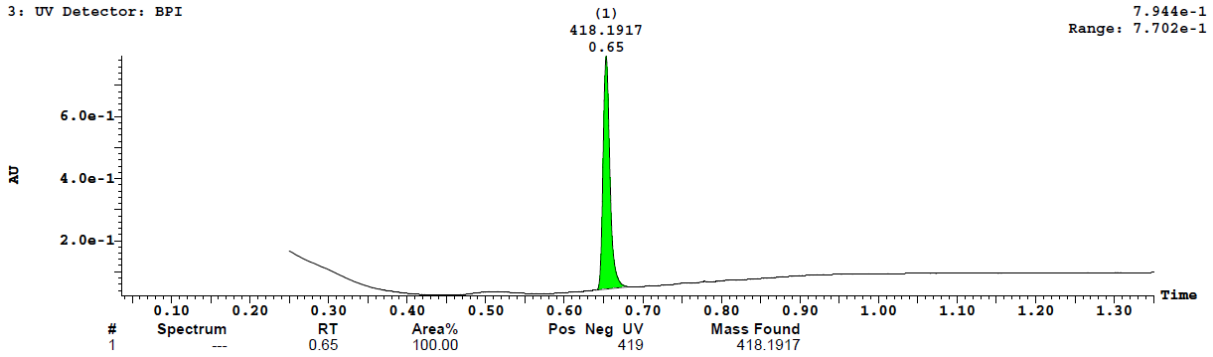
Example 39

LC-MS [Method 4]: R_t = 0.66 min. MS (ESI+): *m/z* = 391.3 $[M+H]^+$.



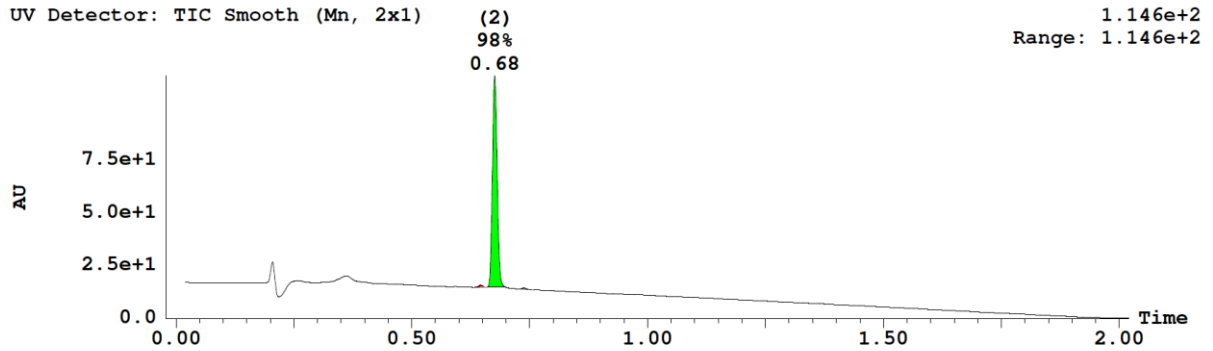
Example 40

LC-MS [Method 4]: R_t = 0.65 min. MS (ESI+): *m/z* = 419.3 $[M+H]^+$.



Example 41

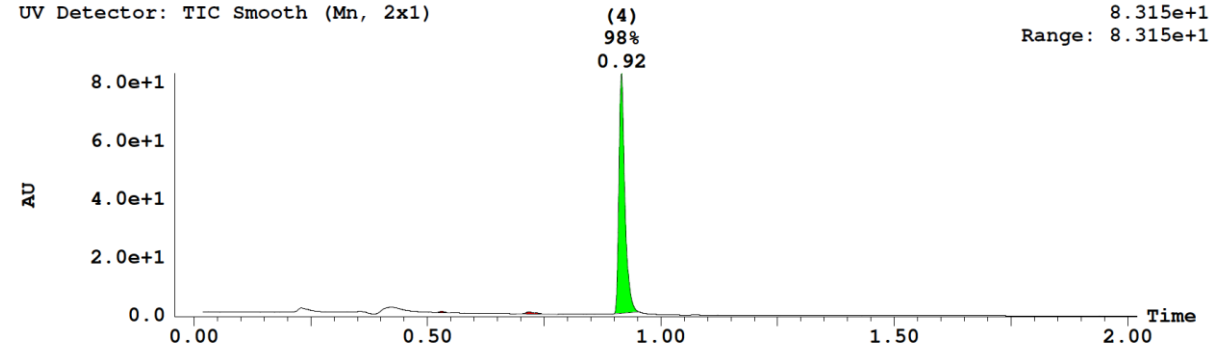
LC-MS [Method 2]: R_t = 0.68 min. MS (ESI+): *m/z* = 464.1 $[M+H]^+$.



Peak Number	Compound	Time	AreaAbs	Area %Total	Mass Found
1		0.65	10904	0.90	
2	Found	0.68	1192283	98.46	231.60
3	Found	0.74	7766	0.64	231.60, 463.00

Example 42

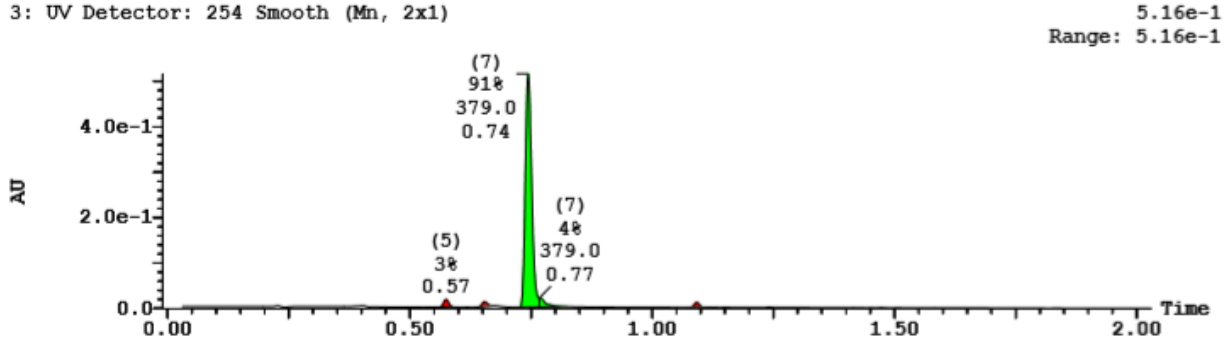
LC-MS [Method 2]: R_t = 0.92 min. MS (ESI+): *m/z* = 402.4 $[M+H]^+$.



Peak Number	Compound	Time	AreaAbs	Area %Total	Mass Found
1		0.53	5695	0.45	
2		0.72	10873	0.87	
3		0.73	7458	0.59	
4	Found	0.92	1232605	98.09	401.20

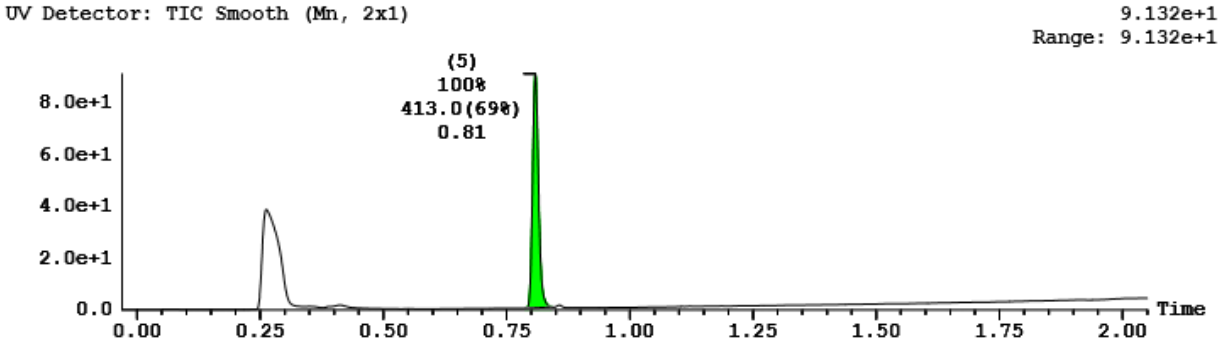
Example 43

LC-MS [Method 1]: R_t = 0.74 min. MS (ESI+): *m/z* = 380.4 $[M+H]^+$.



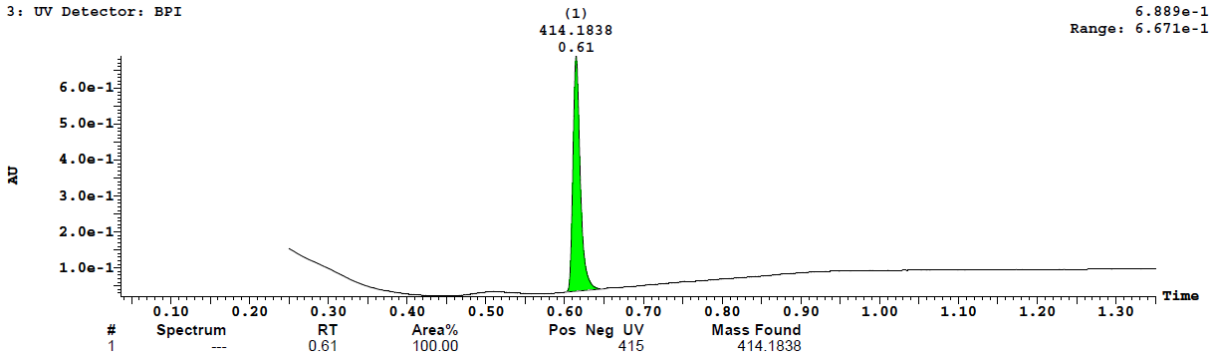
Example 44

LC-MS [Method 1]: R_t = 0.81 min. MS (ESI+): *m/z* = 414.2 $[M+H]^+$.



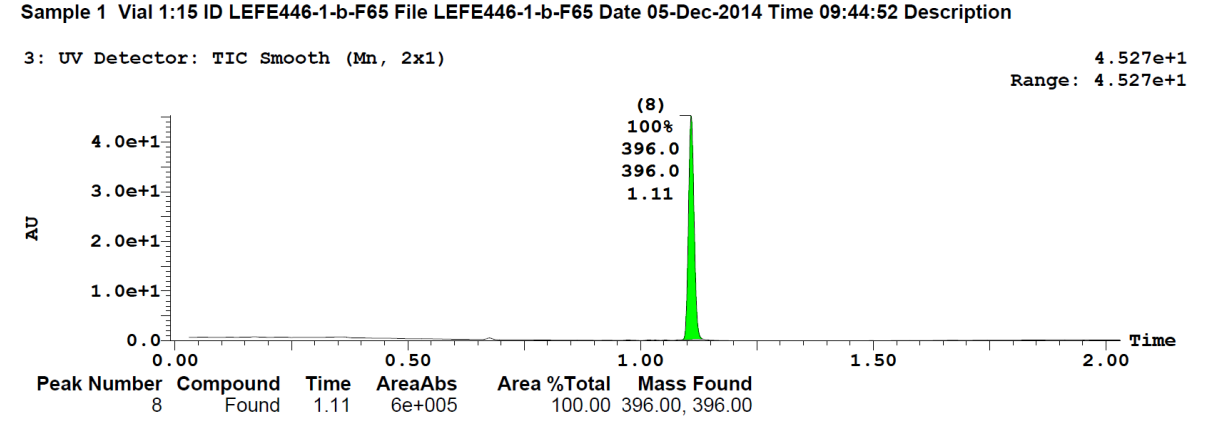
Example 45

LC-MS [Method 4]: R_t = 0.61 min. MS (ESI+): *m/z* = 415.3 $[M+H]^+$.



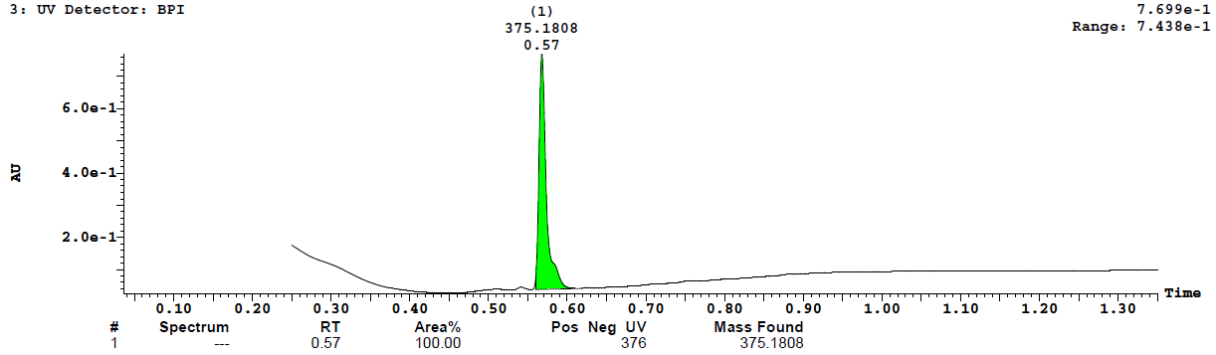
Example 46

LC-MS [Method 2]: R_t = 1.11 min. MS (ESI+): *m/z* = 397.2 $[M+H]^+$.



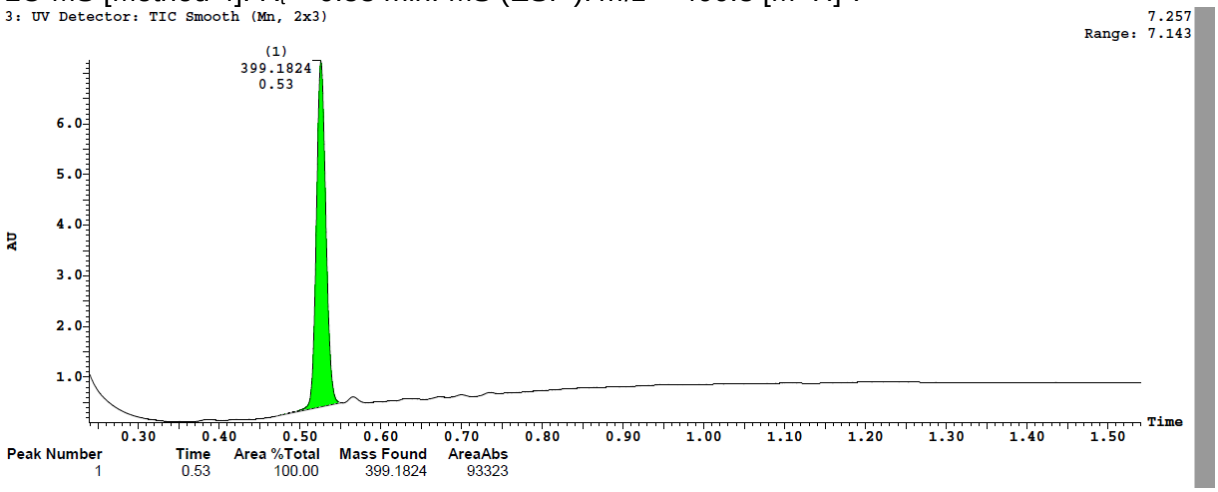
Example 47

LC-MS [Method 4]: R_t = 0.57 min. MS (ESI+): *m/z* = 376.1 $[M+H]^+$.



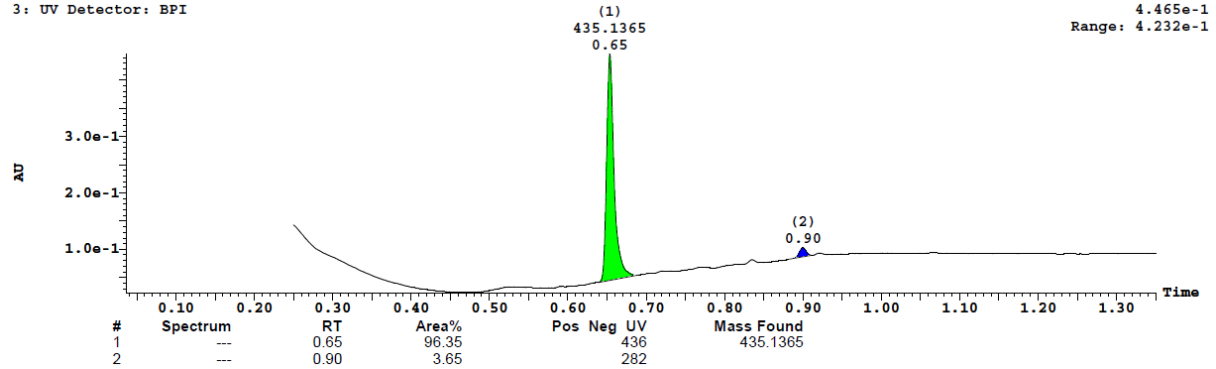
Example 48

LC-MS [Method 4]: R_t = 0.53 min. MS (ESI+): *m/z* = 400.3 $[M+H]^+$.



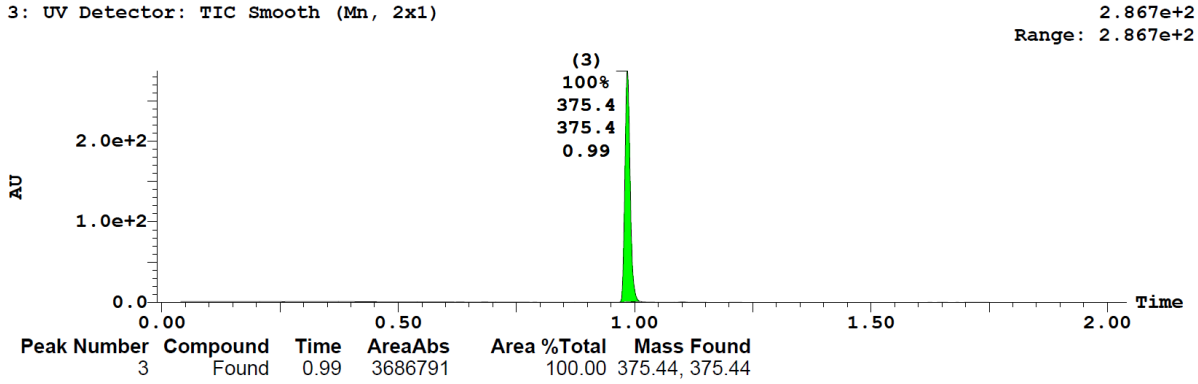
BAY-937

LC-MS [Method 4]: R_t = 0.65 min. MS (ESI+): *m/z* = 436.3 $[M+H]^+$.



BAY 1895344

LC-MS [Method 2]: R_t = 0.99 min. MS (ESI+): *m/z* = 376.1 $[M+H]^+$.



Peak Number	Compound	Time	AreaAbs	Area %Total	Mass Found
3	Found	0.99	3686791	100.00	375.44, 375.44