

Supporting information

Development and utility of a PAK1-Selective Degradar – Supplemental Information

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Co-senior authors

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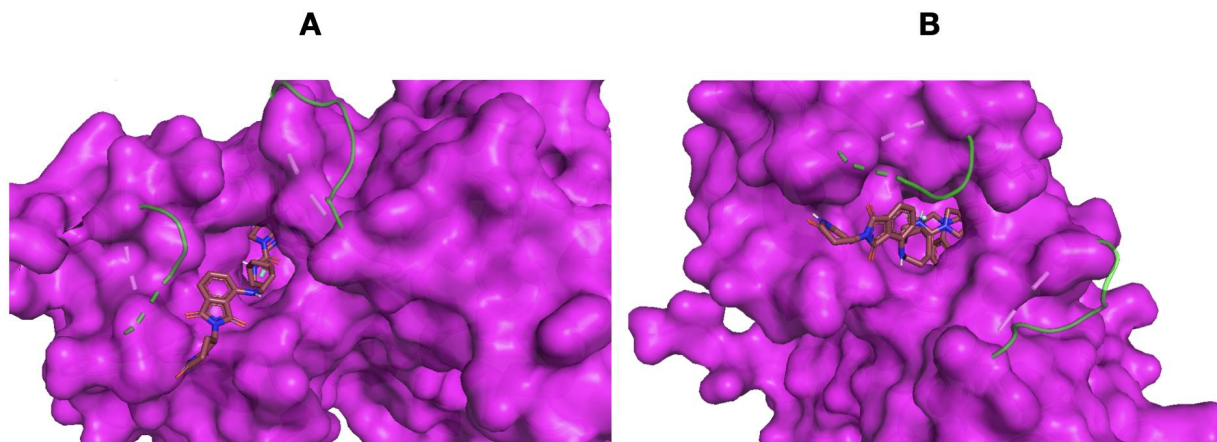
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Experimental Procedures and Characterizations

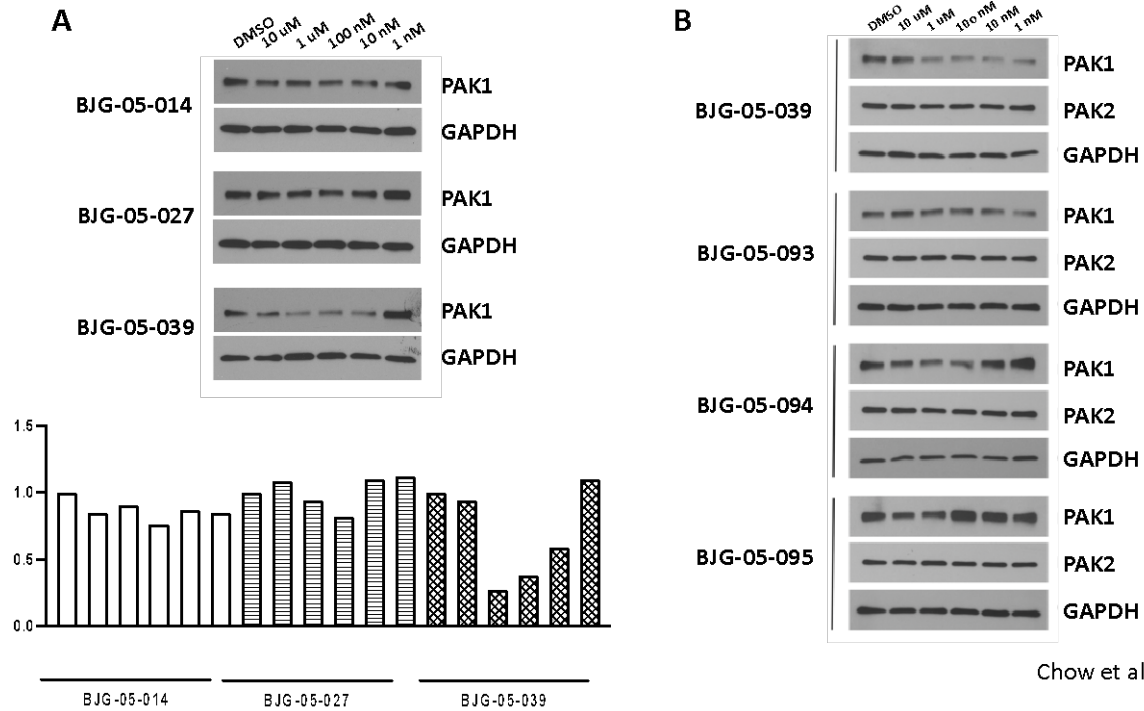
References

Figure S1. Surface representations of PAK1 (PDB: 4ZJI, chain A) and BJJ-05-039 (O=C7CCC(n6c(=O)c5cccc(NCCCCCCCCNC(=O)N4CC[C@@H](Nc2nc1cc(F)ccc1n(CC(F)F)c3ccc(Cl)cc23)C4)c5c6=O)C(=O)N7) docked into the kinase. For clear demonstrations that the ligand occupies ATP pocket region of PAK1, S1A and S1B were taken from 90-degree apart angles. All figures were visualized in PyMOL 2.3.5



Chow et al Figure S1

Figure S2. A) Profiling NVS-based (allosteric) degraders BJG-05-014, BJG-05-027, and BJG-05-039 via western blots in Panc1 cells. Quantification is shown below. B) Profiling NVS-based (allosteric) degrader BJG-05-039 and ATP-competitive degraders BJG-05-093, BJG-05-094, and BJG-05-095 via western blots in Panc1 cells.



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Figure S3. KINOMEscan Profiling of BJK-05-039 @ 10 μ M. Image generated using TREEspot Software Tool and reprinted with permission from KINOMEscan, a division of DiscoverRx Corporation.

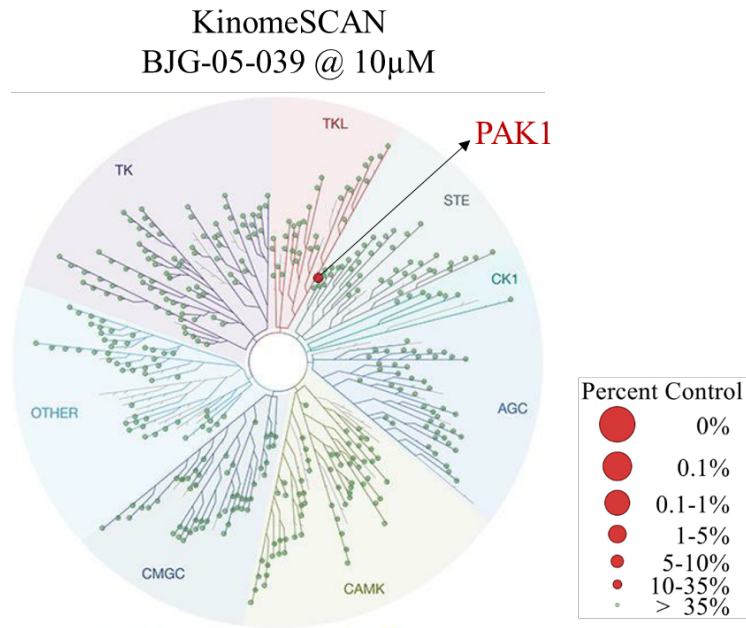
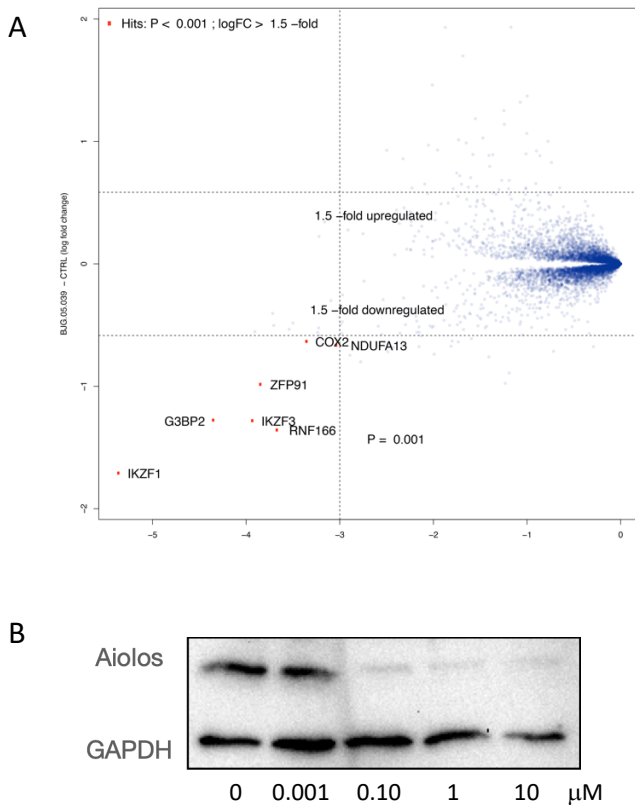
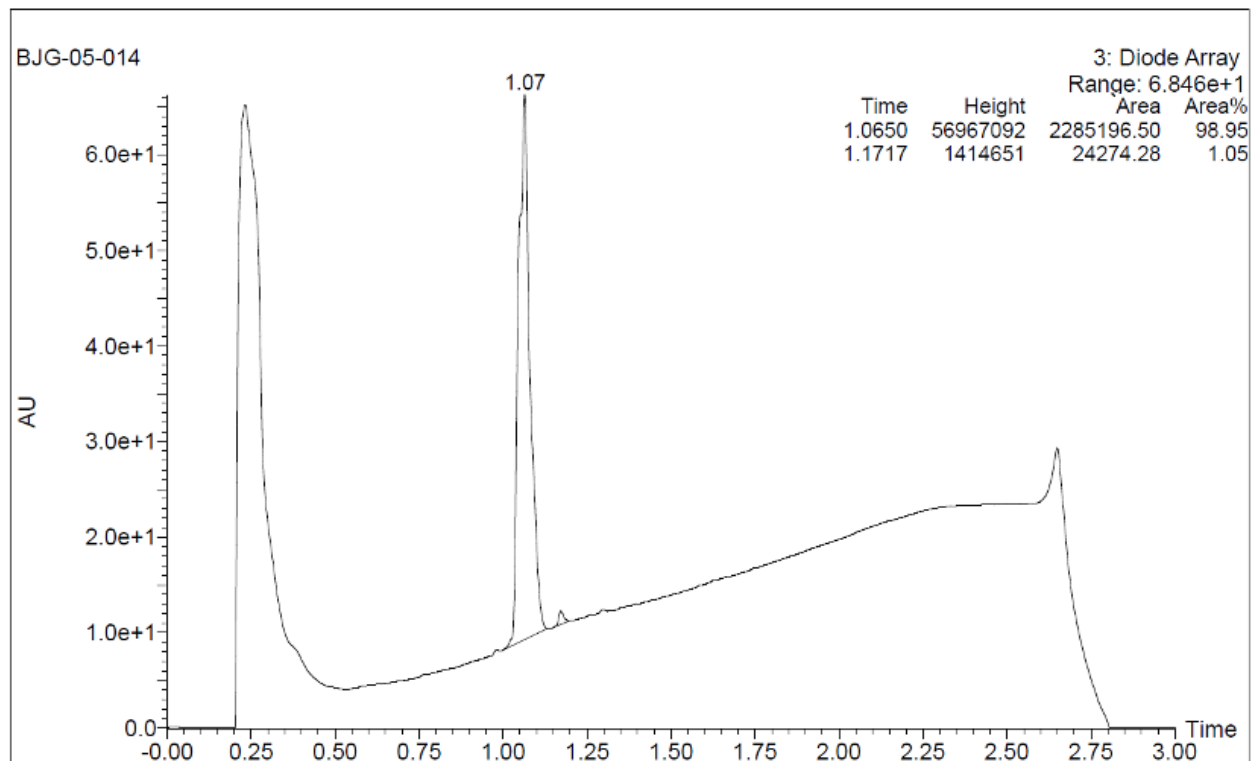


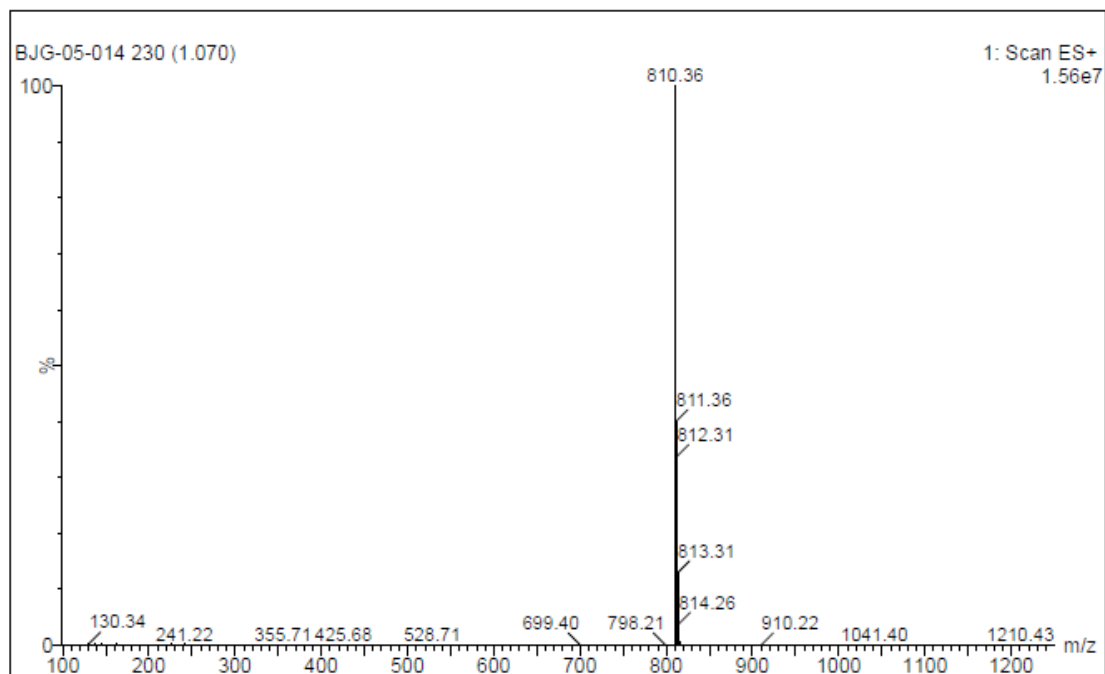
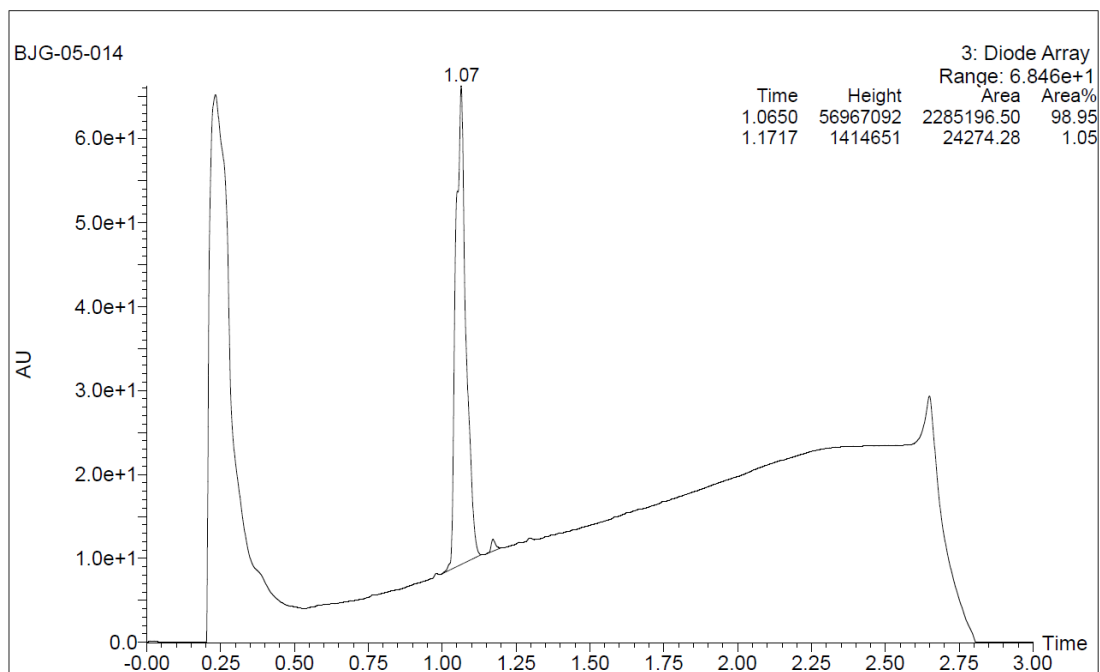
Figure S4. A) Effect of BJJG-05-039 on Proteome. Scatterplot depicts the change in relative protein abundance of MOLT cells treated with BJJG-05-039 (5 h, @ 1 μ M) compared with DMSO vehicle control-treated cells. Protein abundance measurements were made using tandem mass spectrometry and significant changes were assessed by moderated t test as implemented in the limma package (Ritchie et al., 2015). The log₂ fold change (log₂ FC) is shown on the y-axis and negative log₁₀ p value (-log₁₀ p value) on the x-axis for three independent biological replicates of each treatment. B) Immunoblot of Aiolos (*a.k.a.* IKZF3) and GAPDH in MCF-7 cells treated with the indicated concentrations of BJJG-05-039 for 2.5 h.

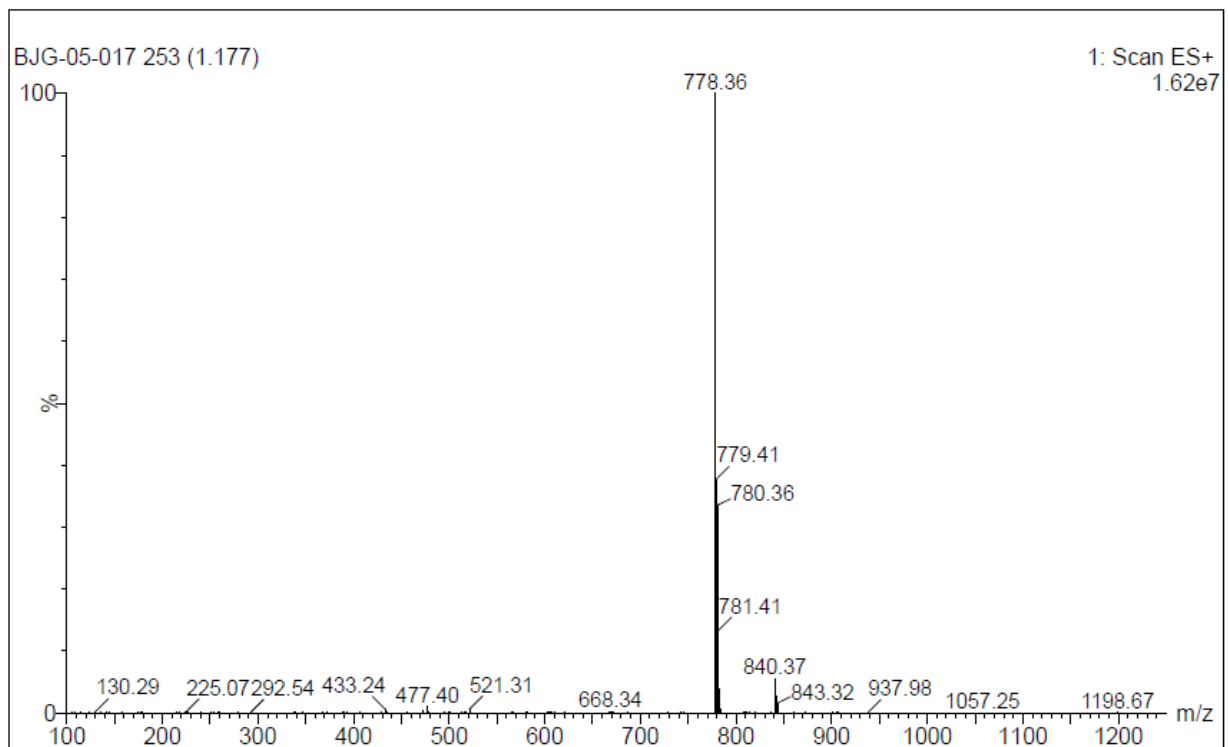
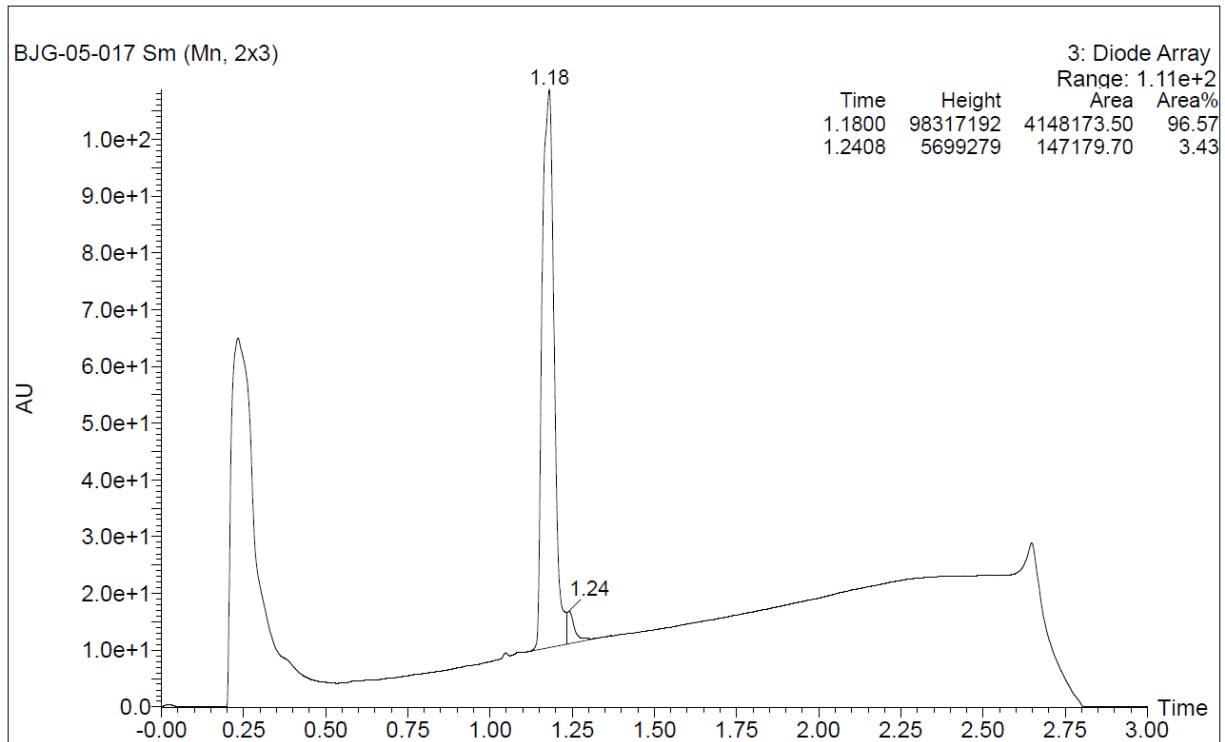


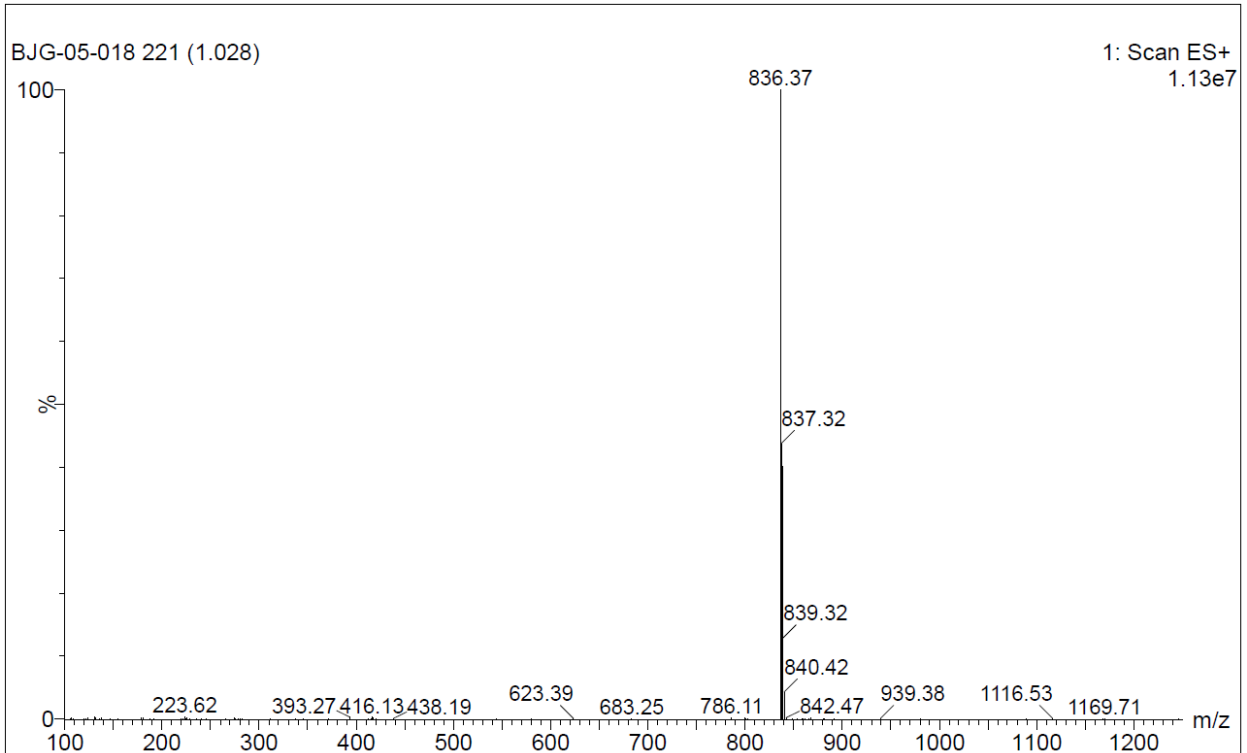
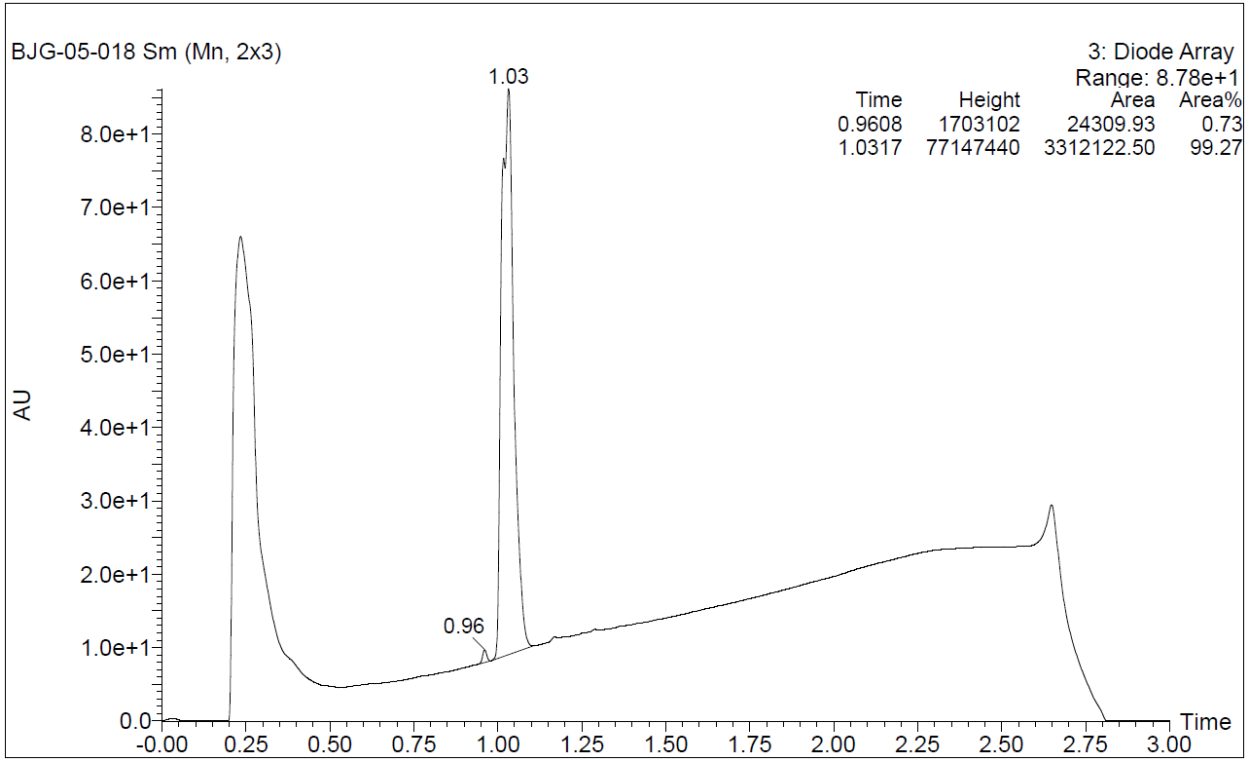
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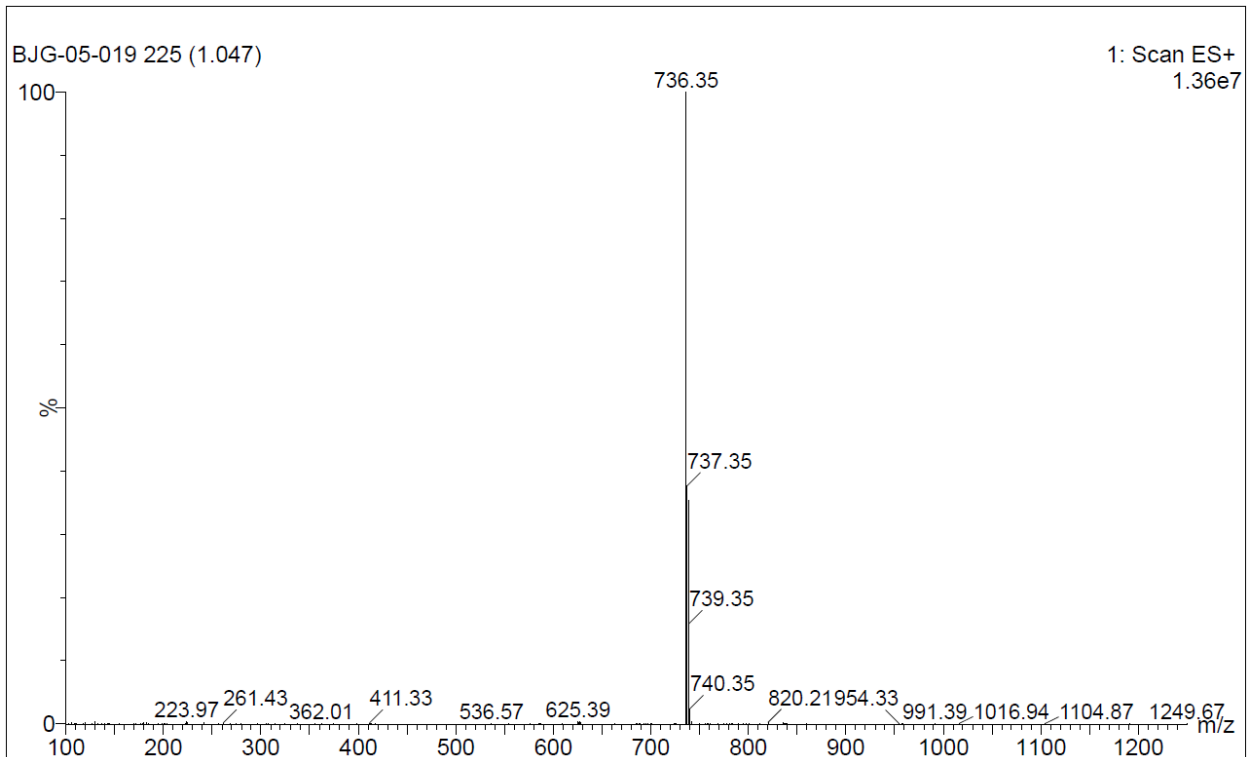
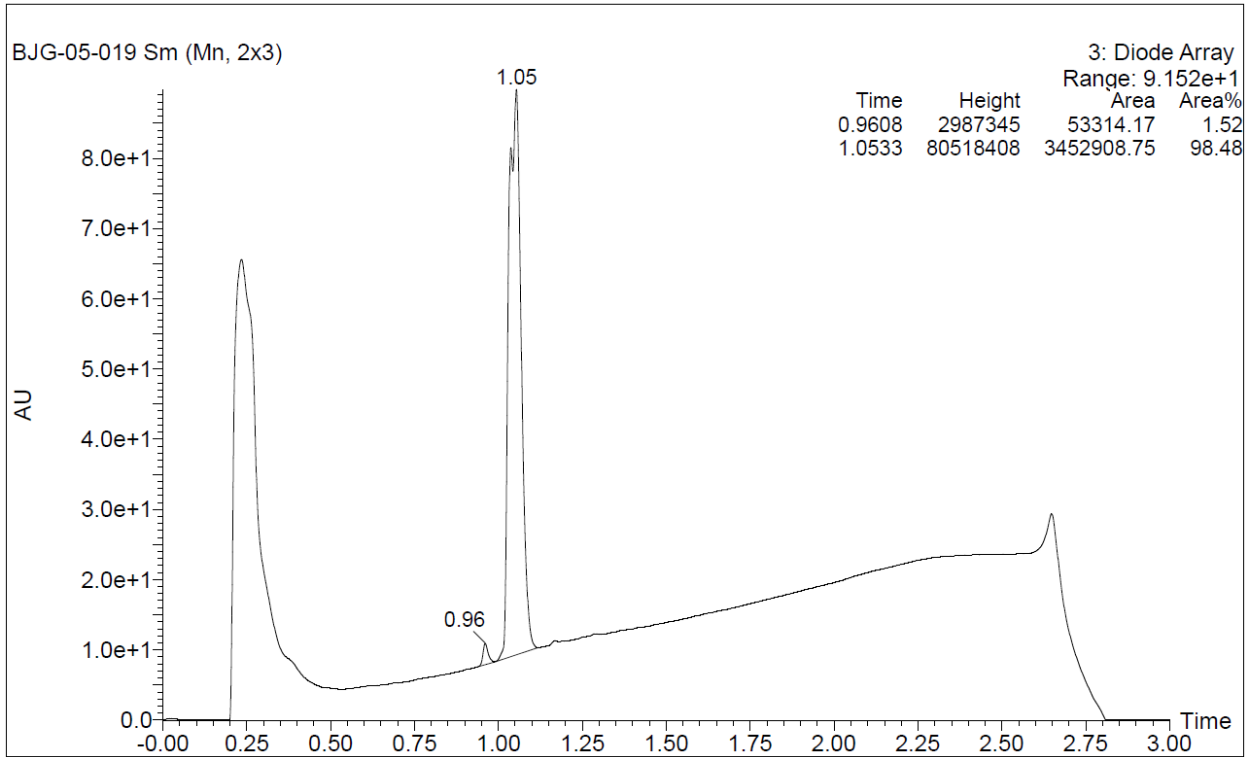
Figure S5. UPLC/MS Spectra

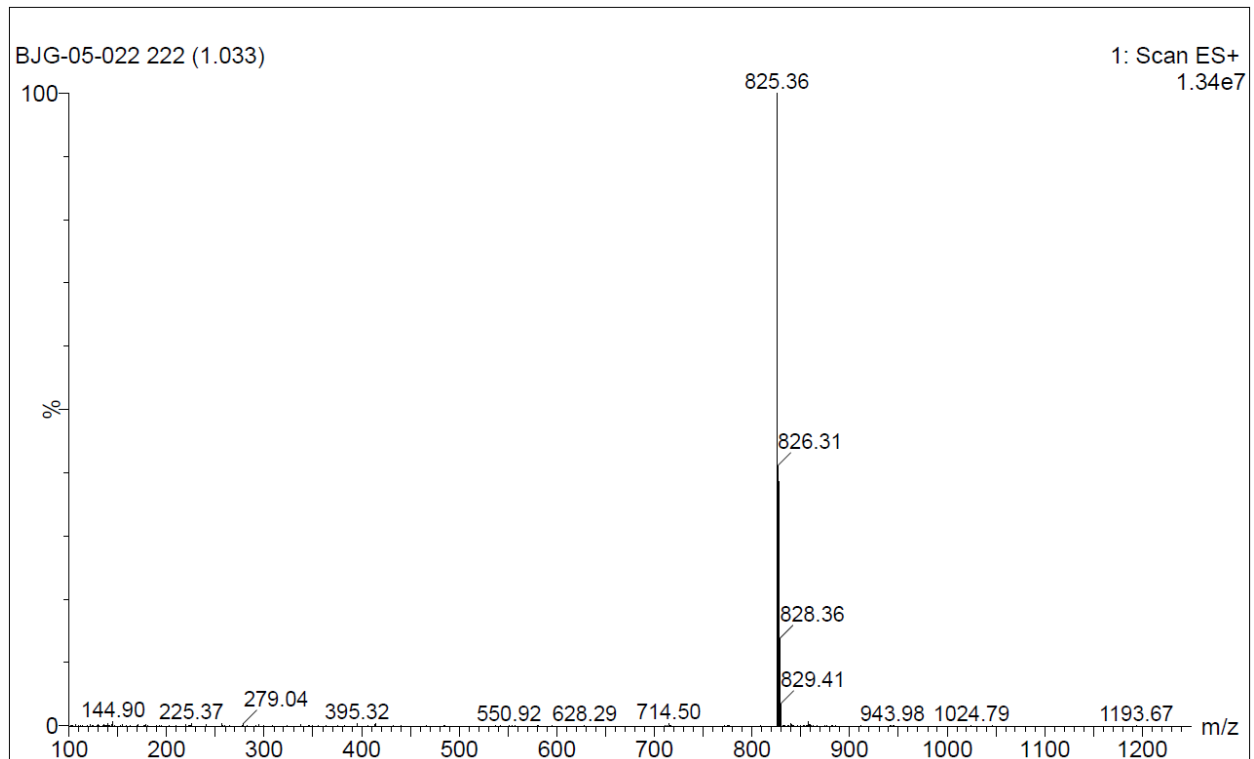
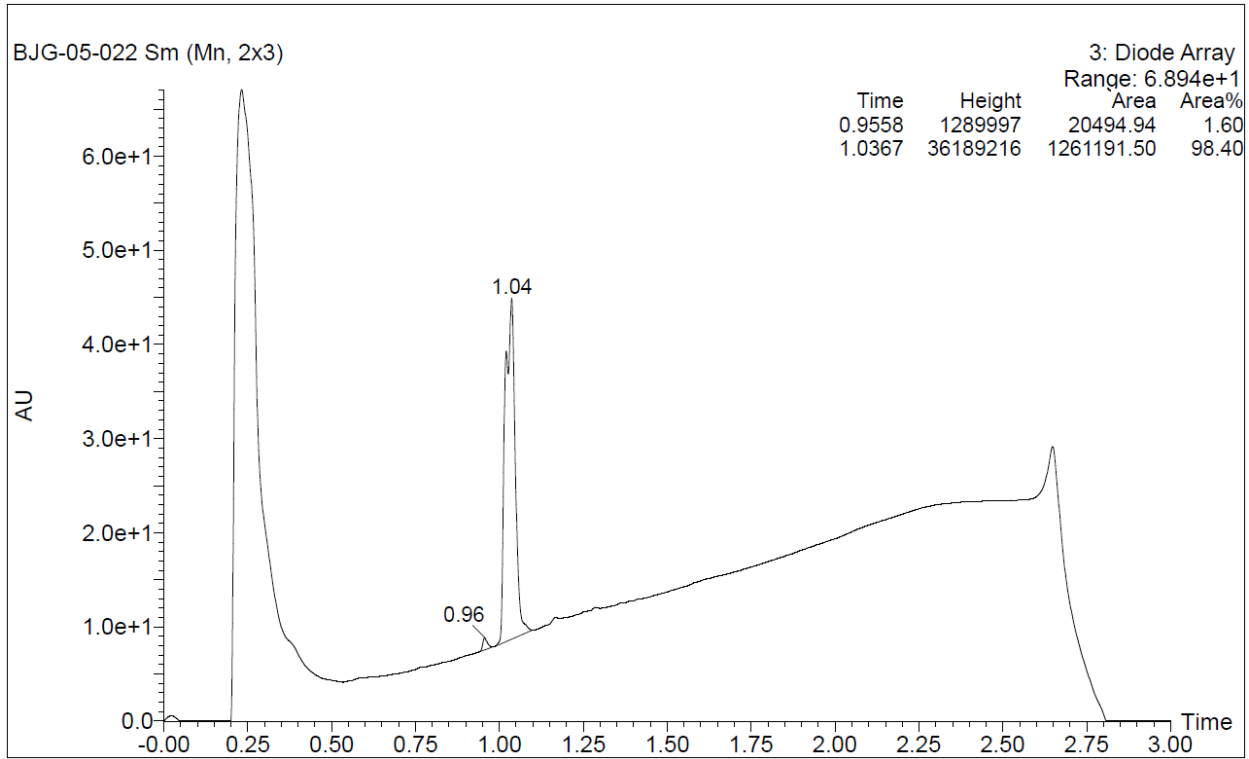


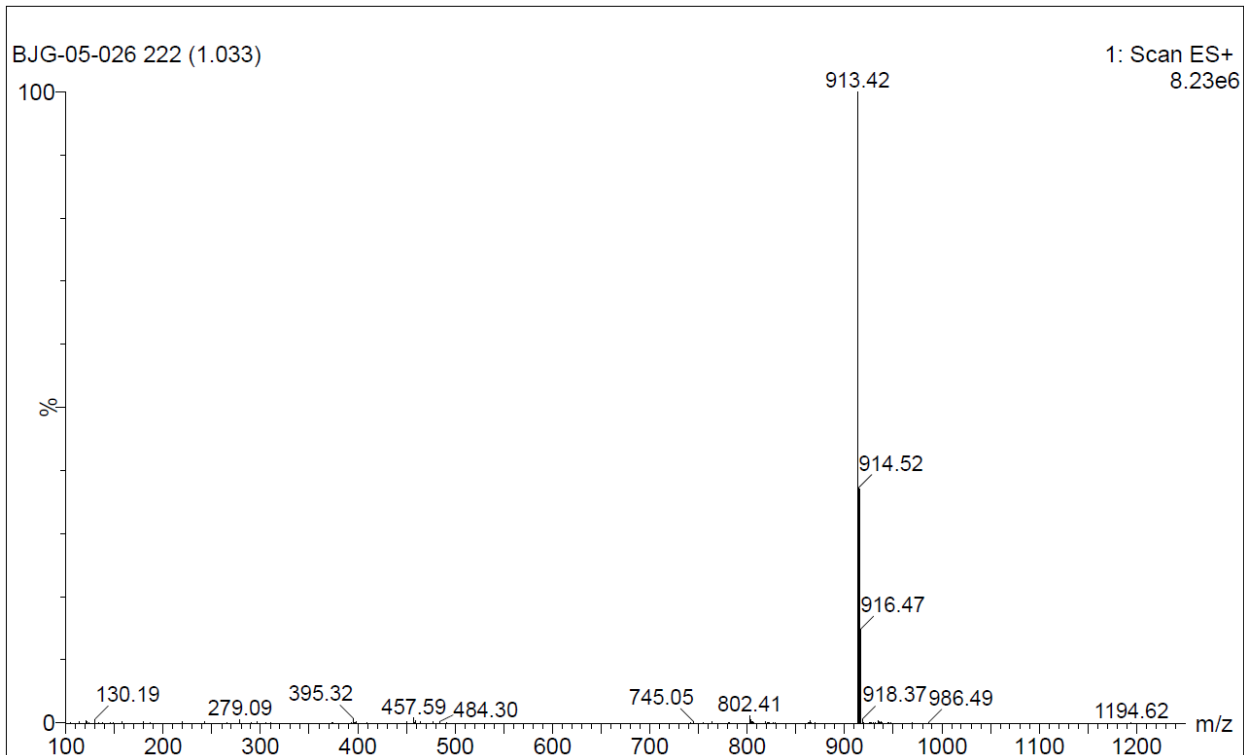
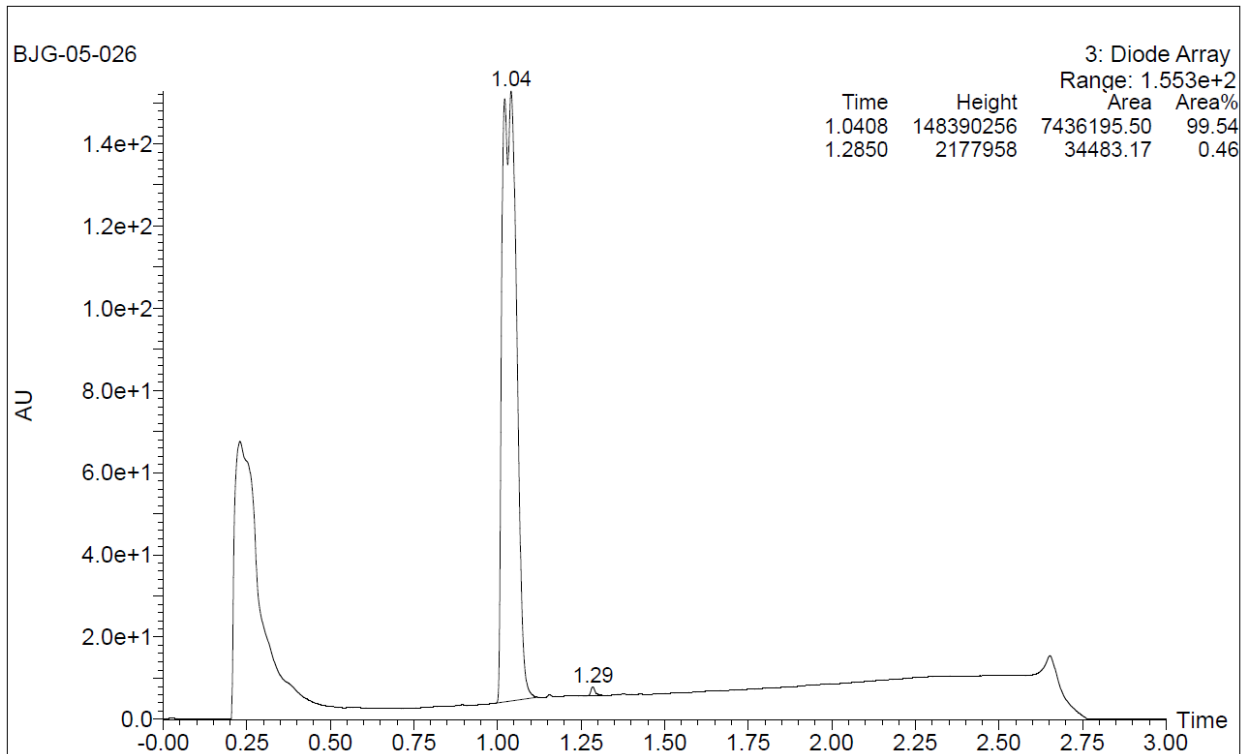


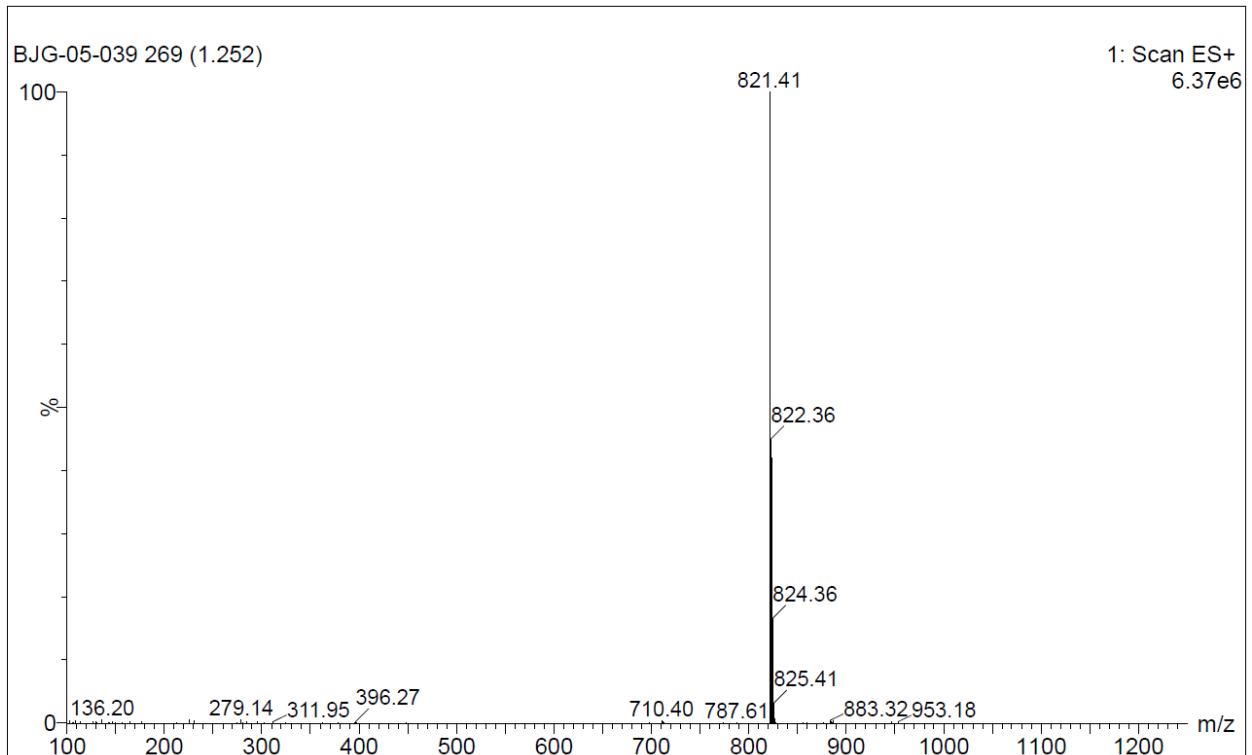
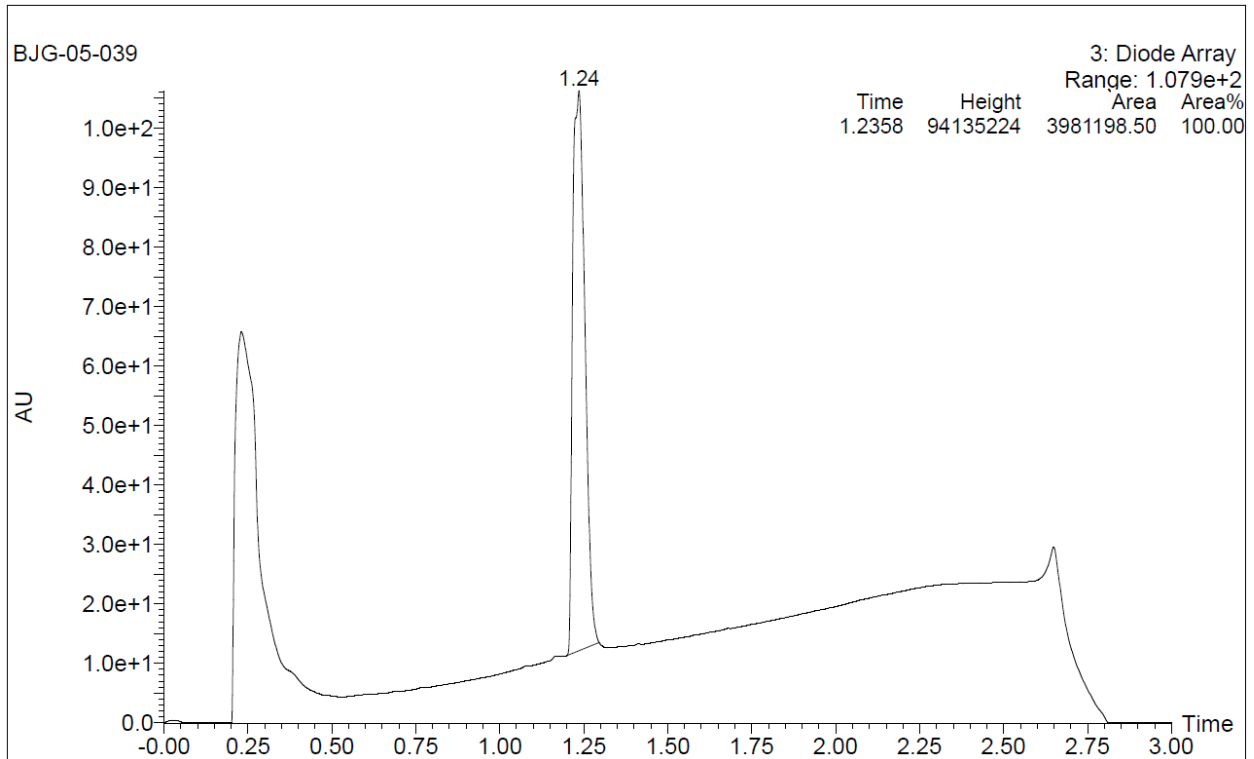


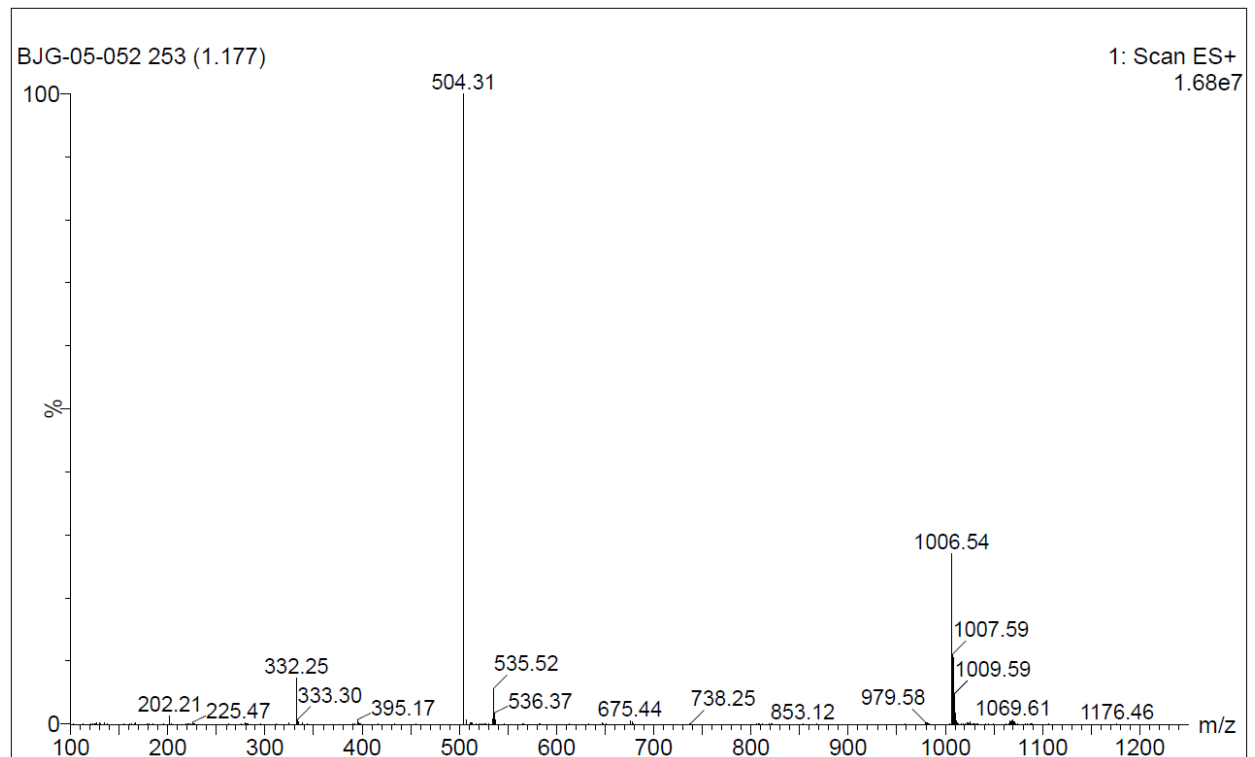
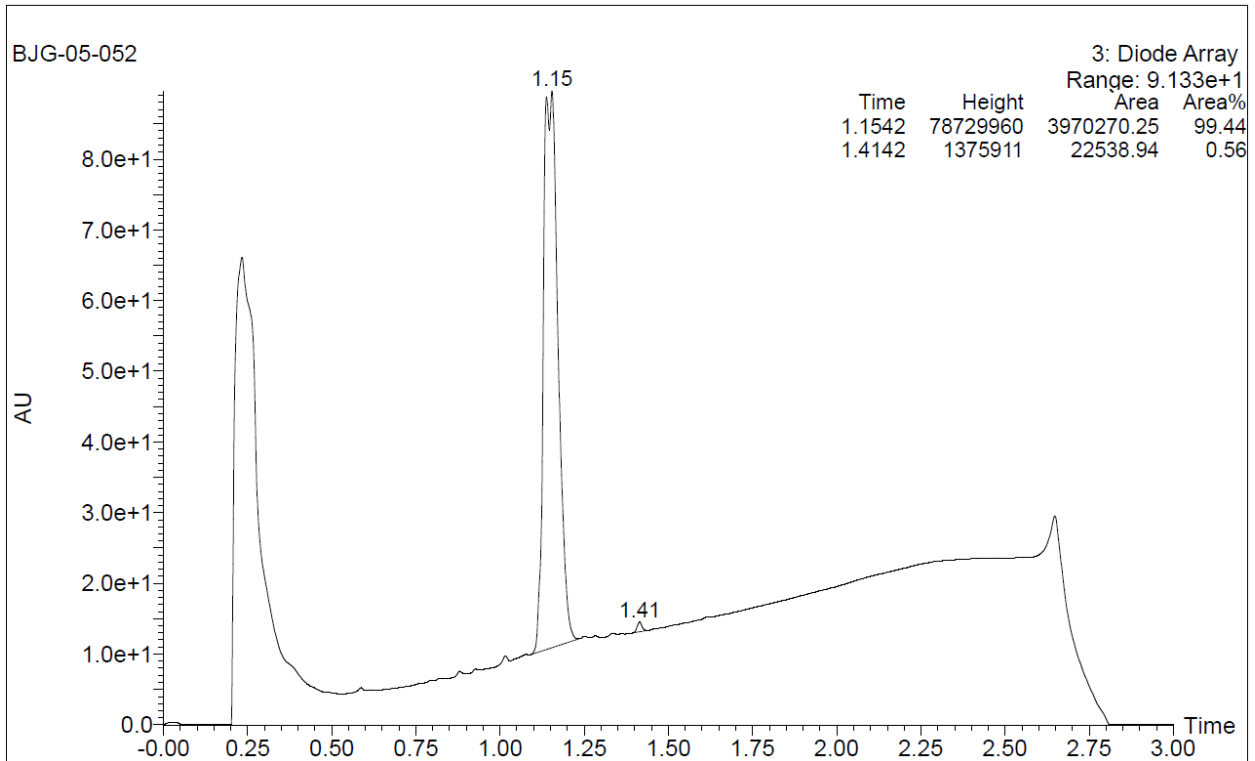


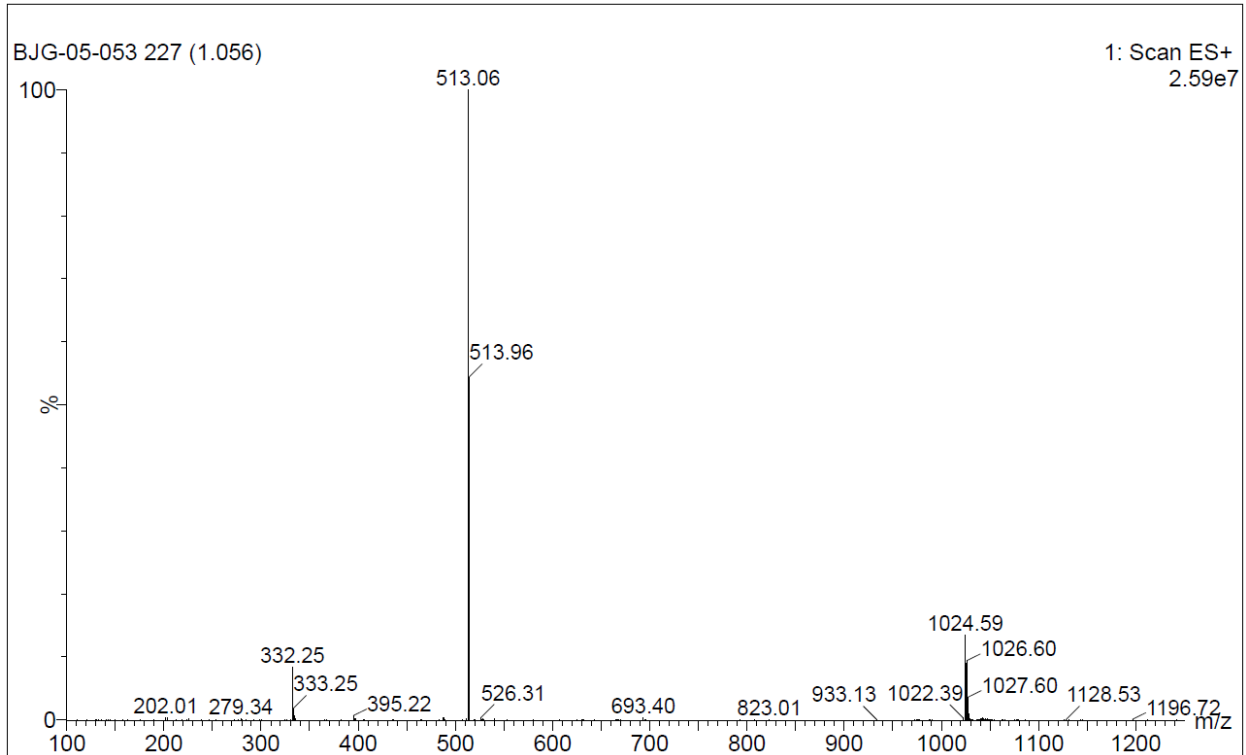
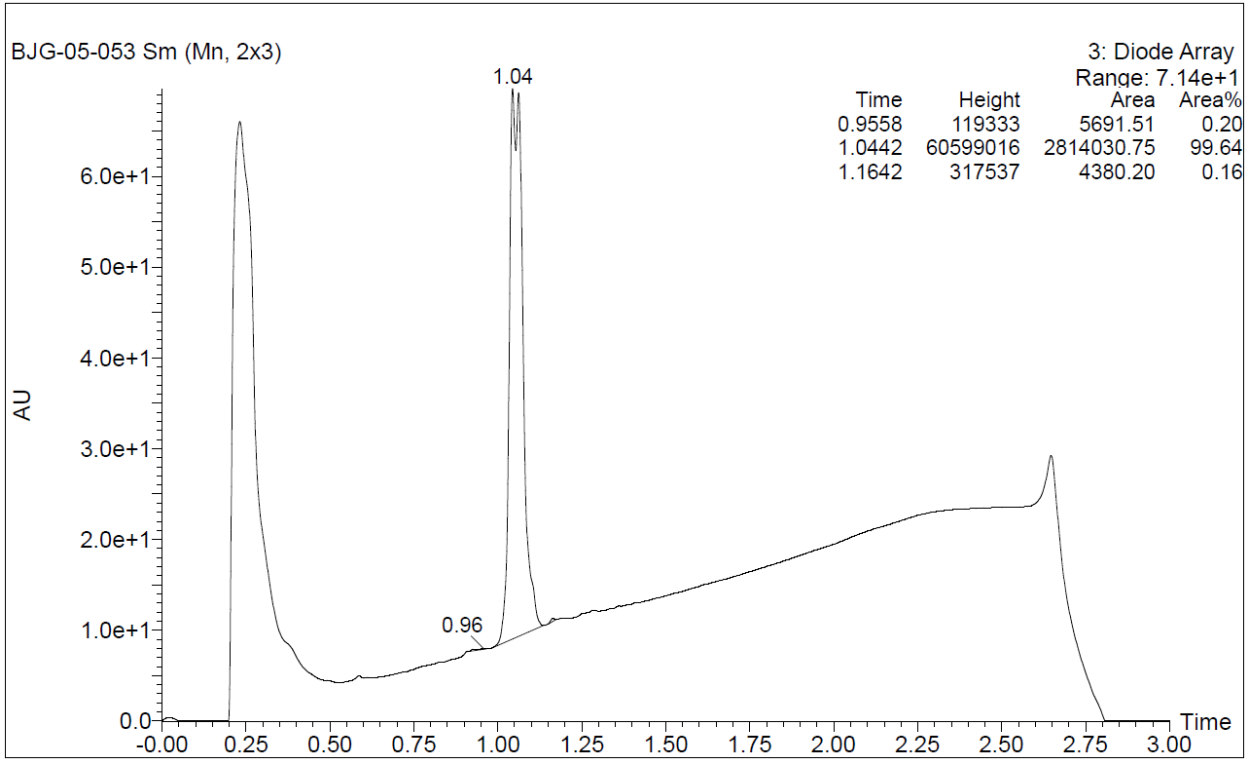


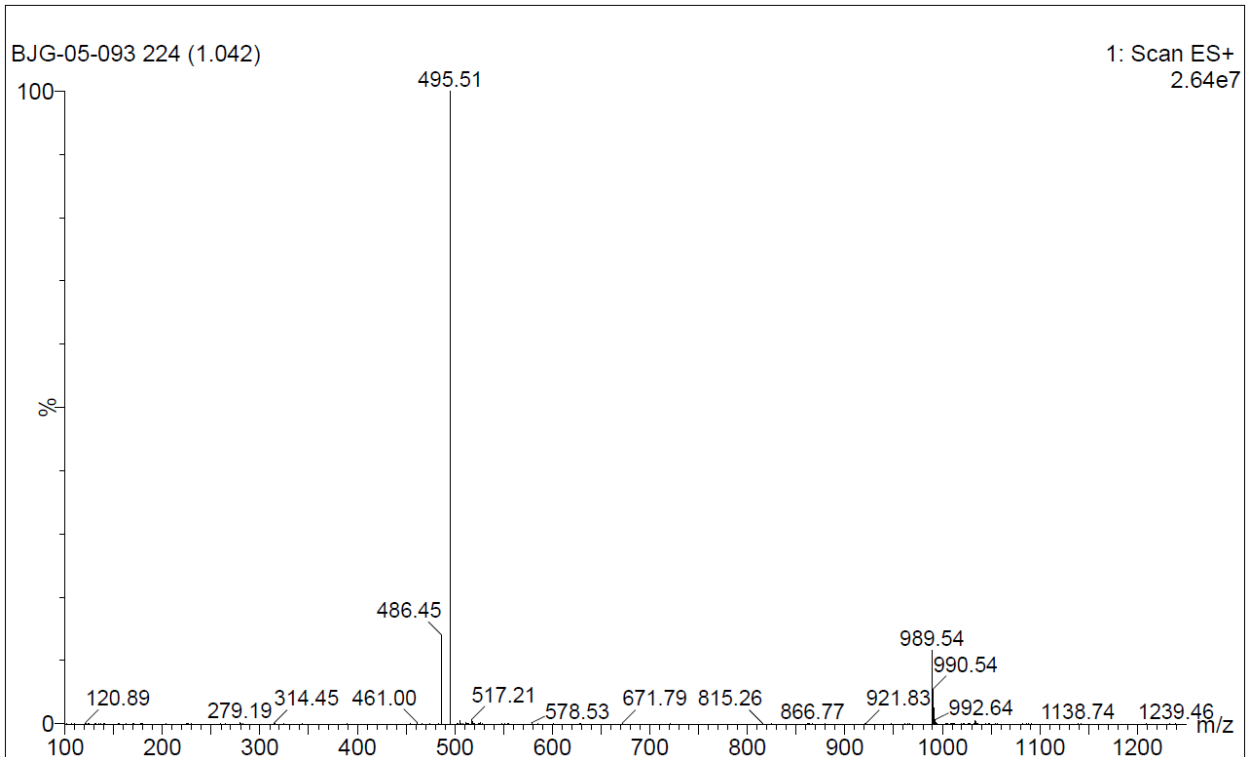
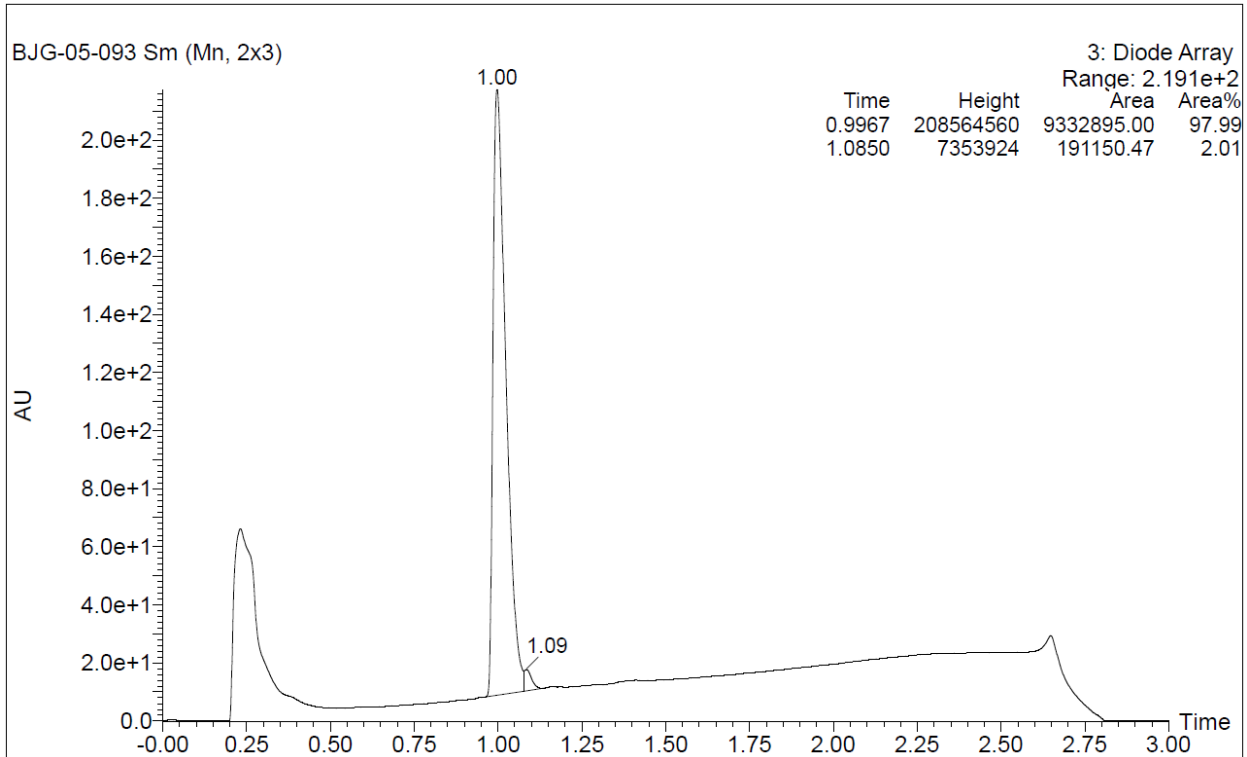


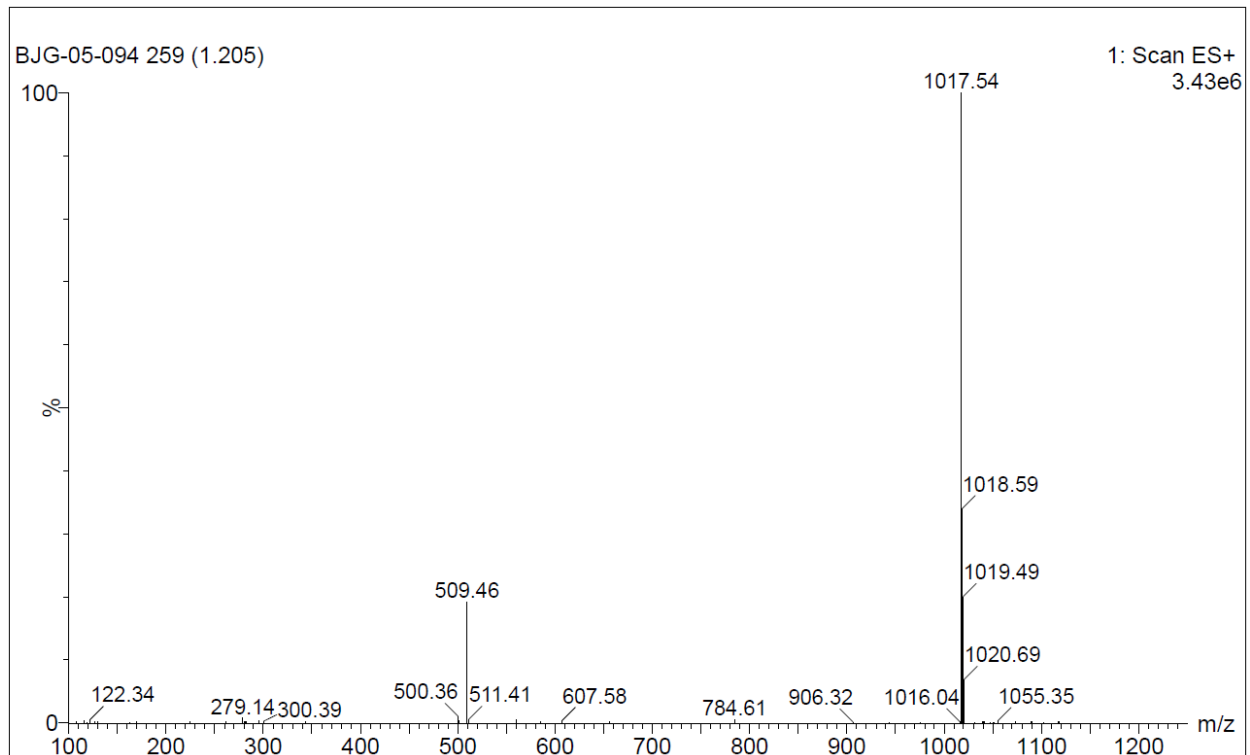
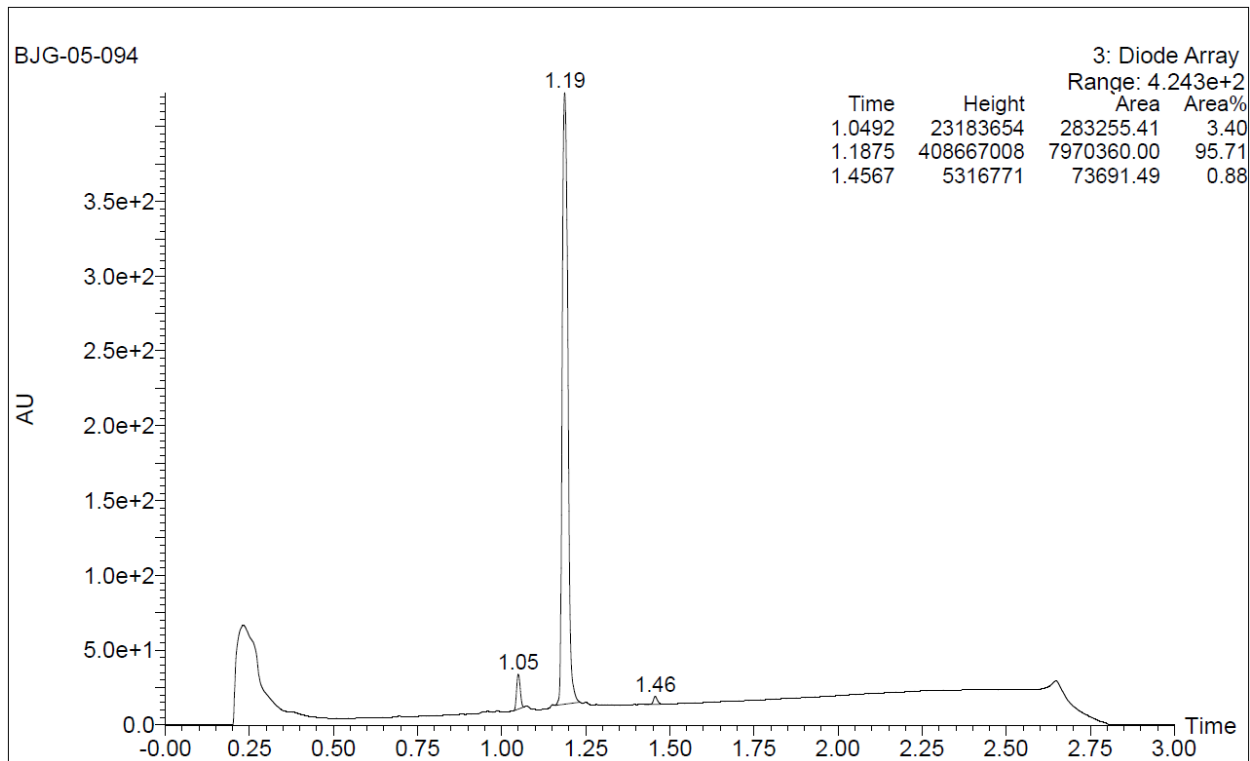












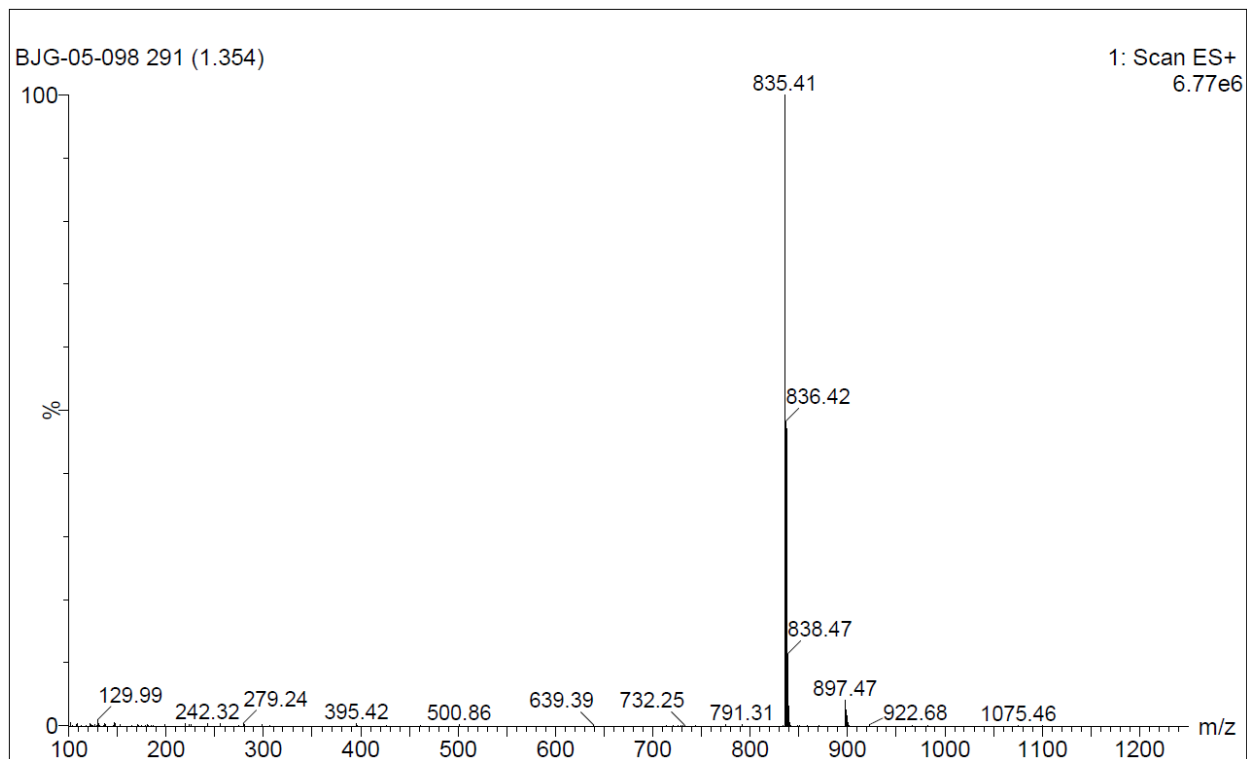
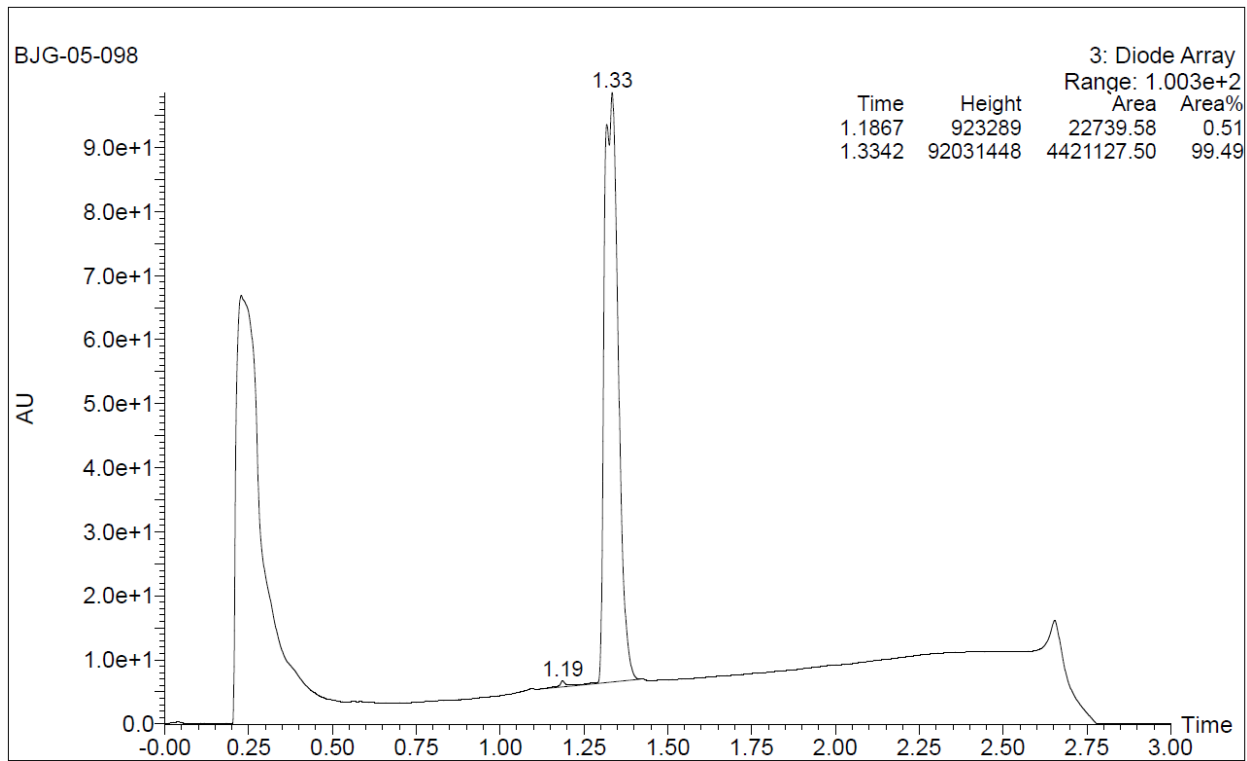
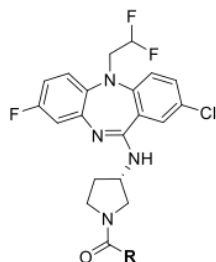
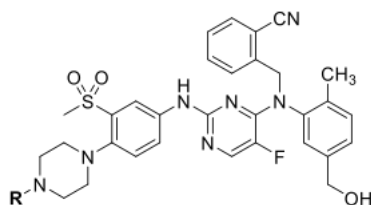


Table S1. Biochemical IC₅₀ data of allosteric PAK1 degraders.



Compound	R	PAK1 IC ₅₀ (nM)	PAK2 IC ₅₀ (nM)	PAK4 IC ₅₀ (nM)
NVS-PAK-1		29.6 ± 3.0	824 ± 84	>10000
BJG-05-014		432 ± 34	724 ± 71	152 ± 13
BJG-05-022		1490 ± 161	6750 ^a	3860 ^a
BJG-05-019		6300 ^a	>10000 ^a	>10000 ^a
BJG-05-017		>1100 ^a	>3300 ^a	>3300 ^a
BJG-05-018		>3300 ^a	>10000 ^a	>10000 ^a
BJG-05-027		594 ± 44	>10000 ^a	>10000 ^a
BJG-05-039		233 ± 19	>10000 ^a	>10000 ^a
BJG-05-020		>10000 ^a	>10000 ^a	>10000 ^a
BJG-05-052		n/a	n/a	n/a
BJG-05-053		n/a	n/a	n/a
BJG-05-098		n/a	n/a	n/a
BJG-05-026		n/a	n/a	n/a

^aThe IC₅₀ for some samples could not be derived because the fitted curves did not reach 50%



Compound	R	PAK1 IC ₅₀ (nM)	PAK2 IC ₅₀ (nM)	PAK4 IC ₅₀ (nM)
BJG-05-093		32.5 ± 3.5	n/a	n/a
BJG-05-094		103 ± 12.1	n/a	n/a
BJG-05-095		36.6 ± 3.3	n/a	n/a

Table S2. KINOMEscan Profiling of BJD-05-039 @ 10 μ M.

BJG-05-039 @ 10 μ M		
DiscoverX Gene Symbol	Entrez Gene Symbol	Percent Control
PAK1	PAK1	20
PRKD3	PRKD3	37
MARK2	MARK2	38
CAMK2A	CAMK2A	39
DAPK3	DAPK3	40
PHKG2	PHKG2	40
DAPK2	DAPK2	41
JAK1(JH1 domain-catalytic)	JAK1	42
PAK7	PAK7	42
RPS6KA5(Kin.Dom.2-C-terminal)	RPS6KA5	42
WEE1	WEE1	42
ARK5	NUAK1	45
CAMK2D	CAMK2D	45
MAP4K4	MAP4K4	45
NDR2	STK38L	45
RSK4(Kin.Dom.2-C-terminal)	RPS6KA6	45
ACVR2B	ACVR2B	46
CAMK2B	CAMK2B	46

CAMKK2	CAMKK2	46
RET	RET	46
TLK1	TLK1	46
DAPK1	DAPK1	47
EPHA3	EPHA3	47
AAK1	AAK1	48
PRKX	PRKX	48
RSK1(Kin.Dom.2-C-terminal)	RPS6KA1	48
TNIK	TNIK	48
AXL	AXL	49
GSK3A	GSK3A	50
ACVR2A	ACVR2A	51
BRSK1	BRSK1	51
CAMK2G	CAMK2G	51
RSK3(Kin.Dom.2-C-terminal)	RPS6KA2	51
CAMK1	CAMK1	52
CAMKK1	CAMKK1	52
CSNK1G1	CSNK1G1	52
DDR1	DDR1	52
DMPK	DMPK	52
ERK4	MAPK4	52
MST3	STK24	52
NEK2	NEK2	52
CDC2L1	CDK11B	53
CDK9	CDK9	53
FLT3	FLT3	53
NLK	NLK	53
PRKD2	PRKD2	53
PKMYT1	PKMYT1	54
IRAK3	IRAK3	55
TTK	TTK	55
GAK	GAK	56
GCN2(Kin.Dom.2,S808G)	EIF2AK4	56
AKT3	AKT3	57
CHEK1	CHEK1	57
CLK1	CLK1	57
ERK5	MAPK7	57
PRKG1	PRKG1	57
DRAK2	STK17B	58
PCTK2	CDK17	58
DRAK1	STK17A	59
ERBB3	ERBB3	59
FLT3(K663Q)	FLT3	59

MAP4K5	MAP4K5	59
RET(V804M)	RET	59
RPS6KA4(Kin.Dom.1-N-terminal)	RPS6KA4	59
CSNK1D	CSNK1D	60
MAPKAPK2	MAPKAPK2	60
MUSK	MUSK	60
p38-alpha	MAPK14	60
PIK3CA	PIK3CA	60
CSNK1E	CSNK1E	61
MET(M1250T)	MET	61
CHEK2	CHEK2	62
CLK3	CLK3	62
PKAC-beta	PRKACB	62
STK16	STK16	62
TIE1	TIE1	62
ADCK4	ADCK4	63
CAMK1G	CAMK1G	63
CSNK1G3	CSNK1G3	63
ERK8	MAPK15	63
FLT3(D835Y)	FLT3	63
KIT(V559D,V654A)	KIT	63
MET(Y1235D)	MET	63
MRCKA	CDC42BPA	63
PIK3CA(H1047L)	PIK3CA	63
ERK3	MAPK6	64
FAK	PTK2	65
INSRR	INSRR	65
NEK5	NEK5	65
PHKG1	PHKG1	65
PKN2	PKN2	65
RIPK1	RIPK1	65
MLCK	MYLK3	66
EGFR(S752-I759del)	EGFR	67
FRK	FRK	67
HIPK4	HIPK4	67
MRCKB	CDC42BPB	67
MYO3A	MYO3A	67
RIPK2	RIPK2	67
TRKB	NTRK2	67
CAMK1D	CAMK1D	68
FGFR4	FGFR4	68
MET	MET	68
CDK2	CDK2	69

IGF1R	IGF1R	70
STK39	STK39	70
ACVRL1	ACVRL1	71
FYN	FYN	71
GRK4	GRK4	71
MAST1	MAST1	71
BRK	PTK6	72
DMPK2	CDC42BPG	72
LIMK2	LIMK2	72
MAP4K3	MAP4K3	72
PKNB(M.tuberculosis)	pknB	72
TRKA	NTRK1	72
TYRO3	TYRO3	72
YANK3	STK32C	72
ASK1	MAP3K5	73
BLK	BLK	73
BUB1	BUB1	73
TSSK1B	TSSK1B	73
BIKE	BMP2K	74
CAMK4	CAMK4	74
CDK3	CDK3	74
CSK	CSK	74
EGFR	EGFR	74
EGFR(L858R)	EGFR	74
EPHB2	EPHB2	74
MTOR	MTOR	74
WNK1	WNK1	74
PAK4	PAK4	75
PIM1	PIM1	75
STK33	STK33	75
TGFBR2	TGFBR2	75
FLT3(D835V)	FLT3	76
MAP3K2	MAP3K2	76
NIK	MAP3K14	76
SGK2	SGK2	76
ABL1(F317L)-nonphosphorylated	ABL1	77
CDKL2	CDKL2	77
DCAMKL1	DCLK1	77
FGFR2	FGFR2	77
GRK2	ADRBK1	77
PIK3CG	PIK3CG	77
PRKCQ	PRKCQ	77
WNK4	WNK4	77

ASK2	MAP3K6	78
CSNK1G2	CSNK1G2	78
CSNK2A2	CSNK2A2	78
EGFR(L747-E749del, A750P)	EGFR	78
PFTAIRE2	CDK15	78
PIK4CB	PI4KB	78
PIM3	PIM3	78
QSK	KIAA0999	78
ULK1	ULK1	78
WEE2	WEE2	78
DCAMKL3	DCLK3	79
LYN	LYN	79
NEK7	NEK7	79
PIKFYVE	PIKFYVE	79
YES	YES1	79
CDK8	CDK8	80
EGFR(L747-T751del,Sins)	EGFR	80
LRRK2	LRRK2	80
MST2	STK3	80
TLK2	TLK2	80
KIT(V559D)	KIT	81
MELK	MELK	81
PRKD1	PRKD1	81
PRKR	EIF2AK2	81
CDC2L5	CDK13	82
EGFR(L747-S752del, P753S)	EGFR	82
EPHA2	EPHA2	82
EPHA4	EPHA4	82
FGR	FGR	82
KIT	KIT	82
LZK	MAP3K13	82
NEK9	NEK9	82
PIM2	PIM2	82
PLK1	PLK1	82
RSK2(Kin.Dom.1-N-terminal)	RPS6KA3	82
SBK1	SBK1	82
STK36	STK36	82
TEC	TEC	82
TNNI3K	TNNI3K	82
ULK2	ULK2	82
ABL1-nonphosphorylated	ABL1	83
ADCK3	CABC1	83
AKT1	AKT1	83

AURKC	AURKC	83
CSNK1A1L	CSNK1A1L	83
EGFR(G719C)	EGFR	83
ERK1	MAPK3	83
FLT3(D835H)	FLT3	83
JNK1	MAPK8	83
MARK3	MARK3	83
MLK1	MAP3K9	83
NEK1	NEK1	83
SgK110	SgK110	83
STK35	STK35	83
TNK1	TNK1	83
YSK1	STK25	83
CDC2L2	CDC2L2	84
EGFR(G719S)	EGFR	84
EPHA8	EPHA8	84
FLT1	FLT1	84
JNK2	MAPK9	84
KIT(L576P)	KIT	84
LTK	LTK	84
RIOK1	RIOK1	84
RIOK3	RIOK3	84
ACVR1B	ACVR1B	85
BMPR1B	BMPR1B	85
CDK11	CDK19	85
ERK2	MAPK1	85
FGFR3	FGFR3	85
KIT(V559D,T670I)	KIT	85
MEK4	MAP2K4	85
PLK4	PLK4	85
PYK2	PTK2B	85
TAOK3	TAOK3	85
ABL1(T315I)-nonphosphorylated	ABL1	86
AKT2	AKT2	86
AMPK-alpha1	PRKAA1	86
CDK4	CDK4	86
DDR2	DDR2	86
EGFR(L858R,T790M)	EGFR	86
FES	FES	86
FLT4	FLT4	86
MEK6	MAP2K6	86
MST4	MST4	86
NDR1	STK38	86

PDGFRB	PDGFRB	86
PDPK1	PDPK1	86
ABL1(Q252H)-nonphosphorylated	ABL1	87
ANKK1	ANKK1	87
CAMK1B	PNCK	87
FLT3(ITD)	FLT3	87
KIT(D816V)	KIT	87
PAK2	PAK2	87
RIPK5	DSTYK	87
RSK1(Kin.Dom.1-N-terminal)	RPS6KA1	87
RSK2(Kin.Dom.2-C-terminal)	RPS6KA3	87
SRPK1	SRPK1	87
EGFR(L861Q)	EGFR	88
FER	FER	88
JNK3	MAPK10	88
MLK3	MAP3K11	88
MYO3B	MYO3B	88
PFTK1	CDK14	88
SGK3	SGK3	88
SRC	SRC	88
ACVR1	ACVR1	89
CSF1R	CSF1R	89
CTK	MATK	89
DYRK2	DYRK2	89
EPHB3	EPHB3	89
GRK1	GRK1	89
LKB1	STK11	89
MAP4K2	MAP4K2	89
NIM1	MGC42105	89
S6K1	RPS6KB1	89
SNRK	SNRK	89
WNK2	WNK2	89
WNK3	WNK3	89
BMX	BMX	90
CDK4-cyclinD1	CDK4	90
CDK5	CDK5	90
EPHA7	EPHA7	90
GSK3B	GSK3B	90
HASPIN	GSG2	90
HCK	HCK	90
MERTK	MERTK	90
MST1	STK4	90
PIK3C2B	PIK3C2B	90

PKAC-alpha	PRKACA	90
RET(M918T)	RET	90
RSK3(Kin.Dom.1-N-terminal)	RPS6KA2	90
TXK	TXK	90
ABL1(F317I)-nonphosphorylated	ABL1	91
EPHB4	EPHB4	91
IKK-alpha	CHUK	91
ITK	ITK	91
LCK	LCK	91
NEK6	NEK6	91
PCTK3	CDK18	91
PIK3CA(E542K)	PIK3CA	91
SLK	SLK	91
SRPK2	SRPK2	91
TYK2(JH1 domain-catalytic)	TYK2	91
DCAMKL2	DCLK2	92
GRK3	ADRBK2	92
HPK1	MAP4K1	92
KIT(A829P)	KIT	92
p38-delta	MAPK13	92
SYK	SYK	92
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TNK2	TNK2	92
ULK3	ULK3	92
AURKB	AURKB	93
CSNK1A1	CSNK1A1	93
ERN1	ERN1	93
INSR	INSR	93
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SRPK3	SRPK3	93
TAOK2	TAOK2	93
YSK4	MAP3K19	93
ABL2	ABL2	94
CIT	CIT	94
EPHA6	EPHA6	94
FLT3(ITD,F691L)	FLT3	94
IKK-beta	IKBKB	94
LIMK1	LIMK1	94
MEK3	MAP2K3	94
MKNK2	MKNK2	94
PIK3CA(H1047Y)	PIK3CA	94
PRKCH	PRKCH	94
ROS1	ROS1	94

RPS6KA5(Kin.Dom.1-N-terminal)	RPS6KA5	94
TRPM6	TRPM6	94
VRK2	VRK2	94
CLK2	CLK2	95
FGFR3(G697C)	FGFR3	95
FLT3(ITD,D835V)	FLT3	95
MAP3K4	MAP3K4	95
PIK3C2G	PIK3C2G	95
PIP5K1A	PIP5K1A	95
PKN1	PKN1	95
RSK4(Kin.Dom.1-N-terminal)	RPS6KA6	95
SIK	SIK1	95
TAOK1	TAOK1	95
CSNK2A1	CSNK2A1	96
LRRK2(G2019S)	LRRK2	96
MEK2	MAP2K2	96
PIP5K1C	PIP5K1C	96
SNARK	NUAK2	96
ALK	ALK	97
EGFR(T790M)	EGFR	97
EPHB6	EPHB6	97
ERBB4	ERBB4	97
FGFR1	FGFR1	97
JAK3(JH1domain-catalytic)	JAK3	97
MLK2	MAP3K10	97
MST1R	MST1R	97
p38-beta	MAPK11	97
PCTK1	CDK16	97
PRKCD	PRKCD	97
PRP4	PRPF4B	97
RAF1	RAF1	97
SIK2	SIK2	97
SRMS	SRMS	97
TYK2(JH2domain-pseudokinase)	TYK2	97
ZAK	ZAK	97
ABL1(H396P)-nonphosphorylated	ABL1	98
BMPR1A	BMPR1A	98
BRAF	BRAF	98
CDKL3	CDKL3	98
EIF2AK1	EIF2AK1	98
EPHA1	EPHA1	98
EPHB1	EPHB1	98
LOK	STK10	98

MAK	MAK	98
MARK1	MARK1	98
PFCDPK1(P.falciparum)	CDPK1	98
RIPK4	RIPK4	98
TIE2	TEK	98
BRSK2	BRSK2	99
CASK	CASK	99
CDKL1	CDKL1	99
EPHA5	EPHA5	99
ICK	ICK	99
JAK2(JH1 domain-catalytic)	JAK2	99
MAP3K15	MAP3K15	99
NEK10	NEK10	99
NEK4	NEK4	99
p38-gamma	MAPK12	99
PAK6	PAK6	99
PLK3	PLK3	99
RET(V804L)	RET	99
RIOK2	RIOK2	99
RPS6KA4(Kin.Dom.2-C-terminal)	RPS6KA4	99
YANK2	STK32B	99
ABL1(E255K)-phosphorylated	ABL1	100
ABL1(F317I)-phosphorylated	ABL1	100
ABL1(F317L)-phosphorylated	ABL1	100
ABL1(H396P)-phosphorylated	ABL1	100
ABL1(M351T)-phosphorylated	ABL1	100
ABL1(Q252H)-phosphorylated	ABL1	100
ABL1(T315I)-phosphorylated	ABL1	100
ABL1(Y253F)-phosphorylated	ABL1	100
ABL1-phosphorylated	ABL1	100
ALK(C1156Y)	ALK	100
ALK(L1196M)	ALK	100
AMPK-alpha2	PRKAA2	100
AURKA	AURKA	100
BMPR2	BMPR2	100
BRAF(V600E)	BRAF	100
BTK	BTK	100
CDK4-cyclinD3	CDK4	100
CDK7	CDK7	100
CDKL5	CDKL5	100
CLK4	CLK4	100
CSF1R-autoinhibited	CSF1R	100
DLK	MAP3K12	100

DYRK1A	DYRK1A	100
DYRK1B	DYRK1B	100
EGFR(E746-A750del)	EGFR	100
ERBB2	ERBB2	100
FLT3(N841I)	FLT3	100
FLT3(R834Q)	FLT3	100
FLT3-autoinhibited	FLT3	100
GRK7	GRK7	100
HIPK1	HIPK1	100
HIPK2	HIPK2	100
HIPK3	HIPK3	100
HUNK	HUNK	100
IKK-epsilon	IKBKE	100
IRAK1	IRAK1	100
IRAK4	IRAK4	100
JAK1(JH2domain-pseudokinase)	JAK1	100
KIT(D816H)	KIT	100
KIT-autoinhibited	KIT	100
LATS1	LATS1	100
LATS2	LATS2	100
MAP3K1	MAP3K1	100
MAP3K3	MAP3K3	100
MAPKAPK5	MAPKAPK5	100
MARK4	MARK4	100
MEK1	MAP2K1	100
MEK5	MAP2K5	100
MINK	MINK1	100
MKK7	MAP2K7	100
MKNK1	MKNK1	100
MYLK	MYLK	100
MYLK4	MYLK4	100
NEK11	NEK11	100
NEK3	NEK3	100
OSR1	OXSRI	100
PAK3	PAK3	100
PDGFRA	PDGFRA	100
PFPK5(P.falciparum)	MAL13P1.279	100
PIK3CA(C420R)	PIK3CA	100
PIK3CA(E545A)	PIK3CA	100
PIK3CA(E545K)	PIK3CA	100
PIK3CA(I800L)	PIK3CA	100
PIK3CA(M1043I)	PIK3CA	100
PIK3CA(Q546K)	PIK3CA	100

PIK3CB	PIK3CB	100
PIK3CD	PIK3CD	100
PIP5K2B	PIP4K2B	100
PIP5K2C	PIP4K2C	100
PLK2	PLK2	100
PRKCE	PRKCE	100
PRKCI	PRKCI	100
PRKG2	PRKG2	100
ROCK1	ROCK1	100
ROCK2	ROCK2	100
SGK	SGK1	100
TAK1	MAP3K7	100
TBK1	TBK1	100
TGFBR1	TGFBR1	100
TRKC	NTRK3	100
TSSK3	TSSK3	100
VEGFR2	KDR	100
VPS34	PIK3C3	100
YANK1	STK32A	100
ZAP70	ZAP70	100

Table S3. Proteomic data of BJG-05-039 @ 10 μ M for 5 hours in MOLT4 cells.

(See attachment)

Table S4. PAK1 Degraders Characterization Table

(See attachment)

KEY RESOURCES TABLE

REAGENT or RESOURC E	SOURCE	IDENTIFIER
Antibodies		

Rabbit monoclonal anti PAK1	Cell Signaling Technology	Cat# 2602; 1:1000
Rabbit monoclonal anti PAK2	Cell Signaling Technology	Cat# 2608; 1:1000
Rabbit polyclonal anti phospho-PAK1/2/3 (S141)	Invitrogen	Cat# 44-940G; 1:1000
Rabbit anti ERK1/2	Cell Signaling Technology	Cat# 4695; 1:2500
Rabbit anti phospho-ERK1/2 (T202/Y204)	Cell Signaling Technology	Cat# 9101; 1:2500
Rabbit anti MEK1/2	Cell Signaling Technology	Cat# 9122; 1:1000
Rabbit anti Aiolos	Cell Signaling Technology	Cat #12720; 1:1000
Rabbit anti phospho-MEK1 (S298)	Cell Signaling Technology	Cat# 9128; 1:1000

Rabbit anti GAPDH	Cell Signaling Technology	Cat# 2118; 1:2500
Chemicals, Cloning Materials, Plasmids, Peptides, and Recombinant Proteins		
DMSO	Fisher	Cat# BP231-100
Bortezomib (PS-341)	Selleckchem	Cat# S1013
Lenalidomide (CC-5013)	Selleckchem	Cat# S1029
NVS-PAK1-1	Sigma-Aldrich	Cat# SML1867
Valspodar	Sigma-Aldrich	Cat# SML0572
DMEM Medium	Gibco	Cat# 10566-016
RPMI Medium	Gibco	Cat# 72400-047
Fetal Bovine Serum	HyClone	Cat# SH30071.03
Penicillin Streptomycin	Gibco	Cat# 15150-122
PAK1 Protein	This study	NA

PAK2 Protein	This study	NA
Doxycycline Hyclate	Sigma-Aldrich	Cat# D9891-1G
Viral Boost Reagent	Alstem	Cat# VB100
Lipofectamine™ 3000	Invitrogen	Cat# L3000001
EcoRI restriction enzyme	NEB	Cat# R3101
XhoI restriction enzyme	NEB	Cat# R0146
In-Fusion HD Enzyme	Takara	Cat# 639649
Stellar competent cells	Takara	Cat# 636766
pFN31K-Nluc	Promega	Cat# N1321
pFN31K-Nluc-PAK1	This study	NA
pLenti-BFP	[Budagyan, 2021 #661]	NA

pCMV6M-Pak1	Addgene	Cat# 12209
Nano-Glo® Endurazine™ Live Cell Substrate	Promega	Cat# N2570/1/2
Critical Commercial Assays		
Z-Lyte (PAK1)	Invitrogen	PV2830
Z-Lyte (PAK2)	Invitrogen	PV4565
Deposited Data		
BGY-05-039 Proteomics in MOLT4 cells	This study	Pride: PXcccc
Experimental Models: Cell Lines		
MOLT4	ATCC	CRL-1582; RRID: CVCL_0013
HEK293	ATCC	CRL-1573; RRID: CVCL_0031

OVCAR3	ATCC	HTB-161; RRID: CVCL_0465
MCF7	ATCC	HTB-22; RRID: CVCL_0031
HeyA8	MDACC	N/A
OMM1	Hans Grossniklaus, Emory University School of Medicine	N/A
Panc1	ATCC	CRL_1469; RRID: CVCL_0480
Software and Algorithms		
GraphPad Prism	GraphPad Software, Inc.	www.graphpad.com/
Adobe Illustrator	Adobe Creative Cloud	https://www.adobe.com/creativecloud.html
Proteome Discoverer 2.2	Thermo Fisher Scientific	https://www.thermofisher.com/order/catalog/product/OPTION-30795

R Framework	Team RCR: A Language and Environment for Statistical Computing	http://www.R-project.org/
Python 3.7.3	Python Software Foundation	https://www.python.org/
SMILES generator	Copyright © 2020 Designed by Themefisher & Developed by Getjekyllthemes	http://www.cheminfo.org/flavor/malaria/Utilities/SMILES_generator___checker/index.html
Open Babel 3.1.0	Copyright (C) 2005-2007 Geoffrey R. Hutchison	https://github.com/openbabel/openbabel/releases
AutoDockTools 1.5.7 AutoDock Vina 1.1.2	designed and implemented by Dr. Oleg Trott in the Molecular Graphics Lab	https://vina.scripps.edu/

SWISS-MODEL	developed by the Computational Structural Biology Group at the SIB Swiss Institute of Bioinformatics	https://swissmodel.expasy.org/

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