Application of large chemical space in an iterative discovery process

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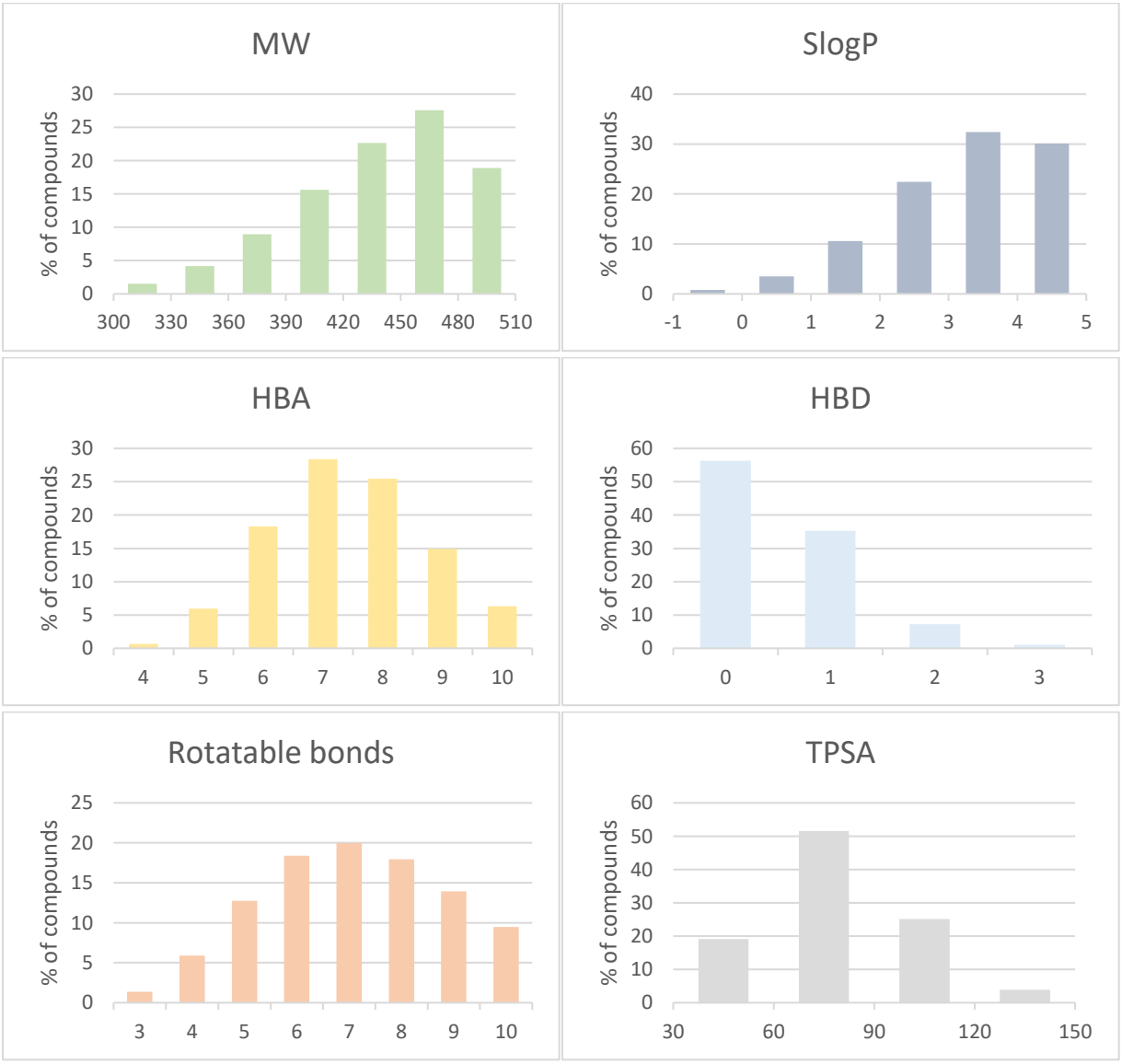
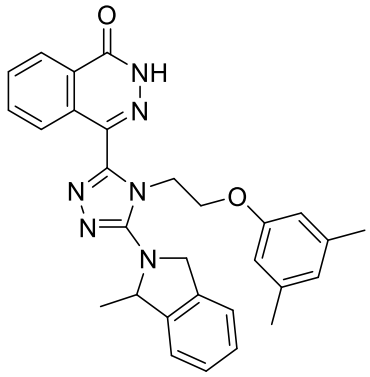
[4]*Enamine Ltd, 78 Chervonotkatska Street, 02094, Ukraine (enamine.net)*

Distribution of PhysChem parameters of the drug-like 221M subset.



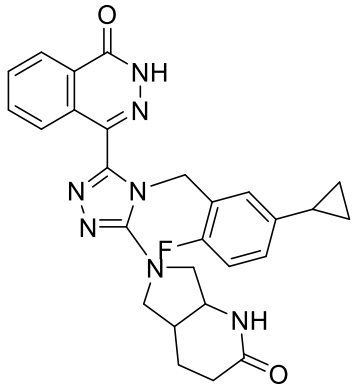
Analytical Data for the synthesized 29 compounds.

4-(4-(2-(3,5-dimethylphenoxy)ethyl)-5-(1-methylisoindolin-2-yl)-4*H*-1,2,4-triazol-3-yl)phthalazin-1(2*H*)-one – 1{1,1,1}



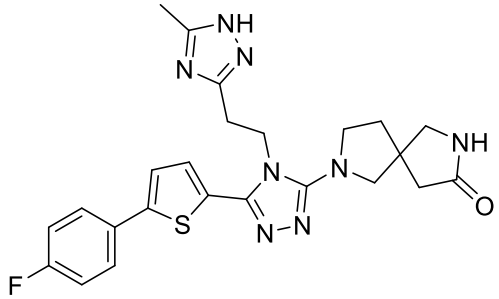
Yield: 32% (64 mg)
LC/MS (APSI) m/z [M+H] calculated for Chemical Formula: $C_{29}H_{28}N_6O_2$: 493.2, found: 493.2.

4-(4-(5-cyclopropyl-2-fluorobenzyl)-5-(2-oxooctahydro-6*H*-pyrrolo[3,4-*b*]pyridin-6-yl)-4*H*-1,2,4-triazol-3-yl)phthalazin-1(2*H*)-one – 1{2,2,1}



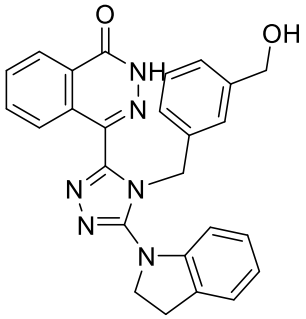
Yield: 18% (35 mg)
LC/MS (APSI) m/z [M+H] calculated for Chemical Formula: $C_{27}H_{26}FN_7O_2$: 500.2, found: 500.1.

7-(5-(5-(4-fluorophenyl)thiophen-2-yl)-4-(2-(5-methyl-1*H*-1,2,4-triazol-3-yl)ethyl)-4*H*-1,2,4-triazol-3-yl)-2,7-diazaspiro[4.4]nonan-3-one – 1{3,3,2}



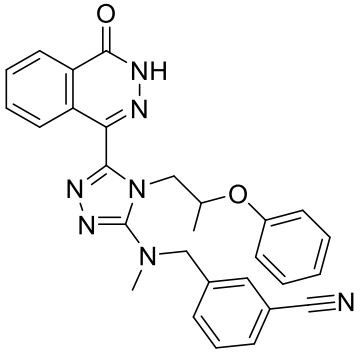
Yield: 46% (98 mg)
LC/MS (APSI) m/z [M+H] calculated for Chemical Formula: $C_{24}H_{25}FN_8OS$: 493.2, found: 493.

4-(4-(3-(hydroxymethyl)benzyl)-5-(indolin-1-yl)-4H-1,2,4-triazol-3-yl)phthalazin-1(2*H*)-one – 1{4,4,1}



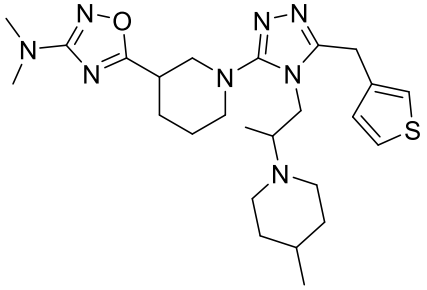
Yield: 42% (86 mg)
LC/MS (APSI) m/z [M+H] calculated for Chemical Formula: $C_{26}H_{22}N_6O_2$: 451.2, found: 451.2.

3-((methyl(5-(4-oxo-3,4-dihydrophthalazin-1-yl)-4-(2-phenoxypropyl)-4*H*-1,2,4-triazol-3-yl)amino)methyl)benzonitrile – 1{5,5,1}



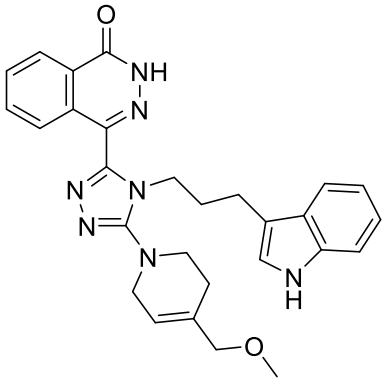
Yield: 36% (65 mg)
LC/MS (APSI) m/z [M+H] calculated for Chemical Formula: $C_{28}H_{25}N_7O_2$: 492.2, found: 492.2.

N,*N*-dimethyl-5-(1-(4-(2-(4-methylpiperidin-1-yl)propyl)-5-(thiophen-3-ylmethyl)-4*H*-1,2,4-triazol-3-yl)piperidin-3-yl)-1,2,4-oxadiazol-3-amine – 1{7,7,4}



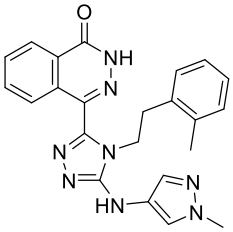
Yield: 64% (135 mg)
LC/MS (APSI) m/z [M+H] calculated for Chemical Formula: $C_{25}H_{38}N_8OS$: 499.3, found: 499.4.

4-(4-(3-(1H-indol-3-yl)propyl)-5-(4-(methoxymethyl)-3,6-dihydropyridin-1(2*H*)-yl)-4*H*-1,2,4-triazol-3-yl)phthalazin-1(2*H*)-one – 1{8,8,1}



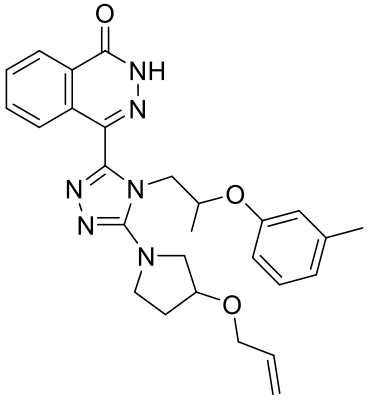
Yield: 52% (108 mg)
LC/MS (APSI) m/z [M+H] calculated for Chemical Formula: $C_{28}H_{29}N_7O_2$: 496.2, found: 496.2.

4-(5-((1-methyl-1H-pyrazol-4-yl)amino)-4-(2-methylphenethyl)-4*H*-1,2,4-triazol-3-yl)phthalazin-1(2*H*)-one – 1{9,9,1}



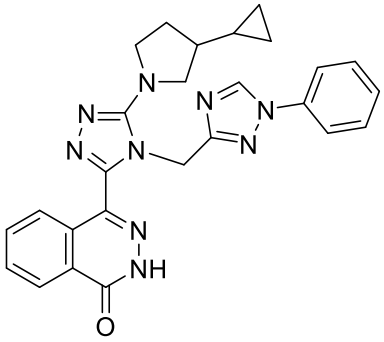
Yield: 58% (115 mg)
LC/MS (APSI) m/z [M+H] calculated for Chemical Formula: $C_{23}H_{22}N_8O$: 427.2, found: 427.
^{1}H NMR (400 MHz, dmso-*d6*) δ 11.77 (s, 1H), 8.94 (s, 1H), 8.21(s, 1H), 7.96 – 7.78 (m, 4H), 7.74 – 7.56 (m, 2H), 7.19 – 7.06 (m, 4H), 4.45 (t, J = 5.6 Hz, 2H), 3.86 (s, 3H), 3.14 – 2.91 (m, 2H), 2.25 (s, 3H).

4-(5-(3-(allyloxy)pyrrolidin-1-yl)-4-(2-(m-tolyloxy)propyl)-4*H*-1,2,4-triazol-3-yl)phthalazin-1(2*H*)-one – 1{10,10,1}



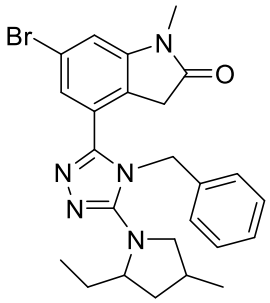
Yield: 38% (73 mg)
LC/MS (APSI) m/z [M+H] calculated for Chemical Formula: $C_{27}H_{30}N_6O_3$: 487.2, found: 487.2.

4-(5-(3-cyclopropylpyrrolidin-1-yl)-4-((1-phenyl-1*H*-1,2,4-triazol-3-yl)methyl)-4H-1,2,4-triazol-3-yl)phthalazin-1(2*H*)-one – 1{12,12,1}



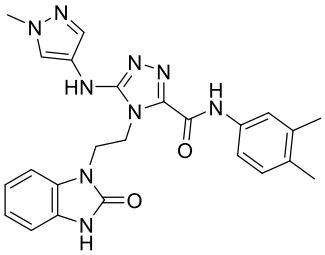
Yield: 16% (32 mg)
LC/MS (APSI) m/z [M+H] calculated for Chemical Formula: $C_{26}H_{25}N_9O$: 480.2, found: 496.2.

4-(4-benzyl-5-(2-ethyl-4-methylpyrrolidin-1-yl)-4*H*-1,2,4-triazol-3-yl)-6-bromo-1-methylindolin-2-one – 1{13,13,6}



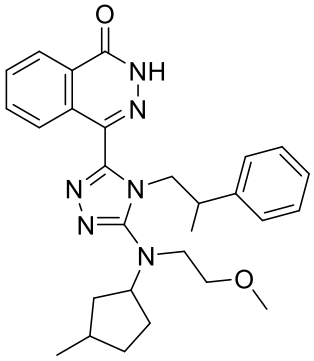
Yield: 30% (60 mg)
LC/MS (APSI) m/z [M+H] calculated for Chemical Formula: $C_{25}H_{28}BrN_5O$: 494.2, found: 494.2.

N-(3,4-dimethylphenyl)-5-((1-methyl-1H-pyrazol-4-yl)amino)-4-(2-(2-oxo-2,3-dihydro-1*H*-benzo[*d*]imidazol-1-yl)ethyl)-4H-1,2,4-triazole-3-carboxamide – 1{16,9,8}



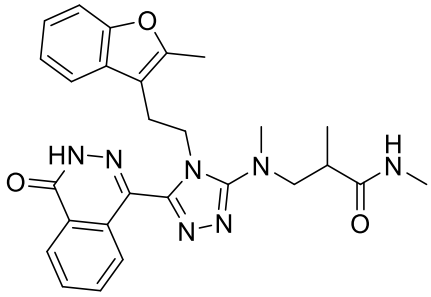
Yield: 31% (62 mg)
LC/MS (APSI) m/z [M-H] calculated for Chemical Formula: $C_{24}H_{25}N_9O_2$: 470.2, found: 470.2.
^{1}H NMR (400 MHz, dmso-*d6*) δ 10.65 (s, 1H), 9.85 (s, 1H), 8.57 (s, 1H), 7.95 (m, 1H), 7.88 (s, 1H), 7.74 – 7.65 (m, 1H), 7.62 – 7.52 (m, 2H), 7.39 – 7.28 (m, 1H), 7.27 – 7.08 (m, 2H), 7.01 – 6.93 (m, 1H), 4.54 – 4.46 (m, 4H), 3.76 (s, 3H), 2.13 (s, 3H), 2.08 (s, 3H).

4-(5-((2-methoxyethyl)(3-methylcyclopentyl)amino)-4-(2-phenylpropyl)-4*H*-1,2,4-triazol-3-yl)phthalazin-1(2*H*)-one – 1{17,17,1}



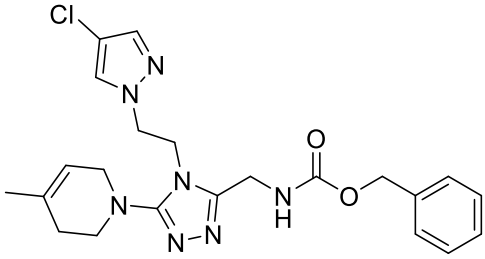
Yield: 26% (51 mg)
LC/MS (APSI) m/z [M+H] calculated for Chemical Formula: $C_{28}H_{34}N_6O_2$: 487.3, found: 487.4.

N,2-dimethyl-3-(methyl(4-(2-(2-methylbenzofuran-3-yl)ethyl)-5-(4-oxo-3,4-dihydrophthalazin-1-yl)-4*H*-1,2,4-triazol-3-yl)amino)propanamide – 1{20,20,1}



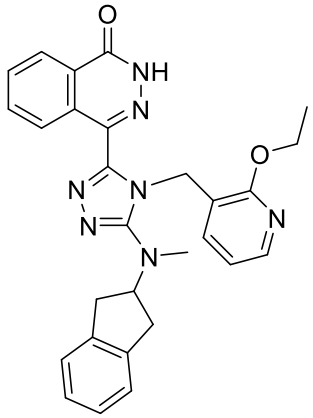
Yield: 48% (101 mg)
LC/MS (APSI) m/z [M+H] calculated for Chemical Formula: $C_{27}H_{29}N_7O_3$: 500.2, found: 500.1.

benzyl ((4-(2-(4-chloro-1H-pyrazol-1-yl)ethyl)-5-(4-methyl-3,6-dihydropyridin-1(2*H*)-yl)-4*H*-1,2,4-triazol-3-yl)methyl)carbamate – 1{21,21,9}



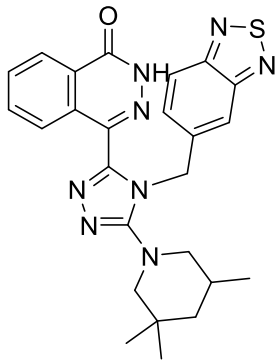
Yield: 25% (63 mg)
LC/MS (APSI) m/z [M+H] calculated for Chemical Formula: $C_{22}H_{26}ClN_7O_2$: 456.2, found: 456.2.

4-(5-((2,3-dihydro-1*H*-inden-2-yl)(methyl)amino)-4-((2-ethoxypyridin-3-yl)methyl)-4*H*-1,2,4-triazol-3-yl)phthalazin-1(2*H*)-one – 1{22,22,1}



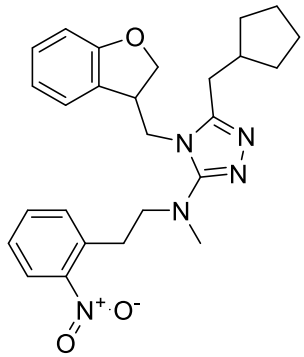
Yield: 60% (121 mg)
LC/MS (APSI) m/z [M+H] calculated for Chemical Formula: $C_{28}H_{27}N_7O_2$: 494.2, found: 494.2.

4-(4-(benzo[*c*][1,2,5]thiadiazol-5-ylmethyl)-5-(3,3,5-trimethylpiperidin-1-yl)-4*H*-1,2,4-triazol-3-yl)phthalazin-1(2*H*)-one – 1{23,23,1}



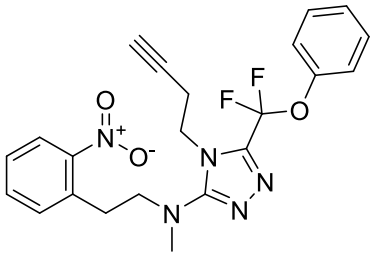
Yield: 59% (115 mg)
LC/MS (APSI) m/z [M+H] calculated for Chemical Formula: $C_{25}H_{26}N_8OS$: 487.2, found: 487.2.

5-(cyclopentylmethyl)-4-((2,3-dihydrobenzofuran-3-yl)methyl)-*N*-methyl-*N*-(2-nitrophenethyl)-4*H*-1,2,4-triazol-3-amine – 1{24,24,10}



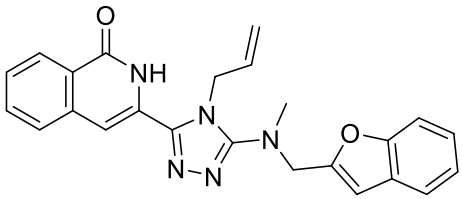
Yield: 22% (44 mg)
LC/MS (APSI) m/z [M+H] calculated for Chemical Formula: $C_{26}H_{31}N_5O_3$: 462.2, found: 462.2.

4-(but-3-yn-1-yl)-5-(difluoro(phenoxy)methyl)-*N*-methyl-*N*-(2-nitrophenethyl)-4*H*-1,2,4-triazol-3-amine – 1{25,24,11}



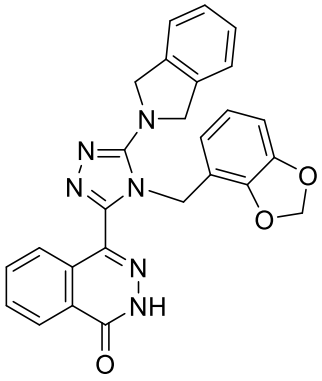
Yield: 28% (56 mg)
LC/MS (APSI) m/z [M+H] calculated for Chemical Formula: $C_{22}H_{21}F_2N_5O_3$: 442.2, found: 442.2.

3-(4-allyl-5-((benzofuran-2-ylmethyl)(methyl)amino)-4H-1,2,4-triazol-3-yl)isoquinolin-1(2*H*)-one – 1{26,25,12}



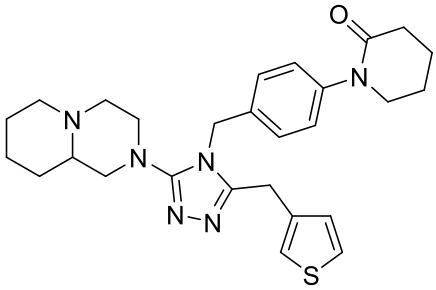
Yield: 55% (106 mg)
LC/MS (APSI) m/z [M+H] calculated for Chemical Formula: $C_{24}H_{21}N_5O_2$: 412.2, found: 412.

4-(4-(benzo[*d*][1,3]dioxol-4-ylmethyl)-5-(isoindolin-2-yl)-4*H*-1,2,4-triazol-3-yl)phthalazin-1(2*H*)-one – 1{28,27,1}



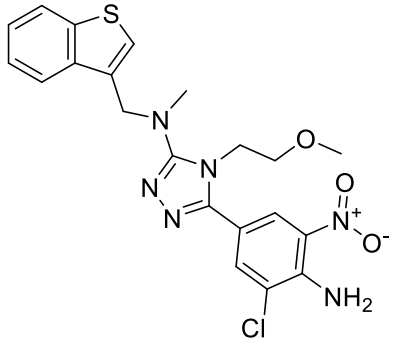
Yield: 58% (112 mg)
LC/MS (APSI) m/z [M+H] calculated for Chemical Formula: $C_{26}H_{20}N_6O_3$: 465.2, found: 465.2.

1-(4-((3-(octahydro-2*H*-pyrido[1,2-*a*]pyrazin-2-yl)-5-(thiophen-3-ylmethyl)-4*H*-1,2,4-triazol-4-yl)methyl)phenyl)piperidin-2-one – 1{29,28,4}



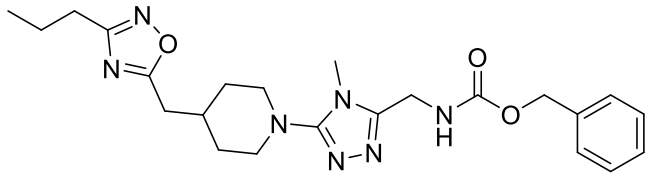
Yield: 35% (106 mg)
LC/MS (APSI) m/z [M+H] calculated for Chemical Formula: $C_{27}H_{34}N_6OS$: 491.3, found: 491.2.

5-(4-amino-3-chloro-5-nitrophenyl)-*N*-(benzo[b]thiophen-3-ylmethyl)-4-(2-methoxyethyl)-*N*-methyl-4*H*-1,2,4-triazol-3-amine – 1{30,29,14}



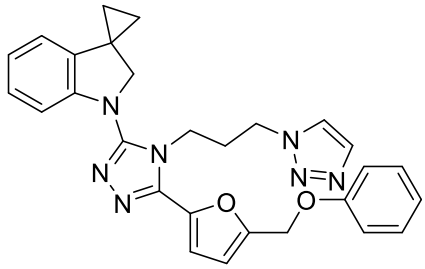
Yield: 53% (92 mg)
LC/MS (APSI) m/z [M+H] calculated for Chemical Formula: $C_{21}H_{21}ClN_6O_3S$: 473.1, found: 473.1.

benzyl ((4-methyl-5-(4-((3-propyl-1,2,4-oxadiazol-5-yl)methyl)piperidin-1-yl)-4*H*-1,2,4-triazol-3-yl)methyl)carbamate – 1{31,30,9}



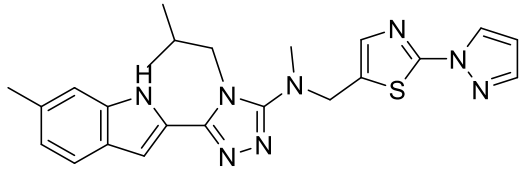
Yield: 35% (67 mg)
LC/MS (APSI) m/z [M+H] calculated for Chemical Formula: $C_{23}H_{31}N_7O_3$: 454.3, found: 454.2.

1'-(4-(3-(1*H*-1,2,3-triazol-1-yl)propyl)-5-(5-(phenoxymethyl)furan-2-yl)-4*H*-1,2,4-triazol-3-yl)spiro[cyclopropane-1,3'-indoline] – 1{32,31,15}



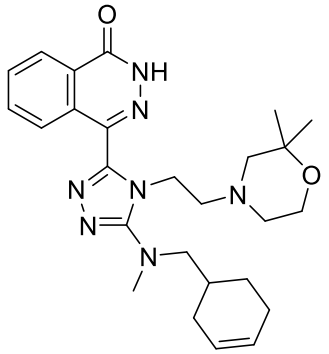
Yield: 42% (87 mg)
LC/MS (APSI) m/z [M+H] calculated for Chemical Formula: $C_{28}H_{27}N_7O_2$: 494.2, found: 494.1.

N-((2-(1*H*-pyrazol-1-yl)thiazol-5-yl)methyl)-4-isobutyl-*N*-methyl-5-(6-methyl-1*H*-indol-2-yl)-4*H*-1,2,4-triazol-3-amine – 1{35,34,16}



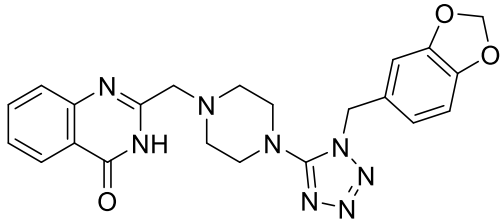
Yield: 56% (111 mg)
LC/MS (APSI) m/z [M-H] calculated for Chemical Formula: $C_{23}H_{26}N_8S$: 445.2, found: 445.2.

4-(5-((cyclohex-3-en-1-ylmethyl)(methyl)amino)-4-(2-(2,2-dimethylmorpholino)ethyl)-4*H*-1,2,4-triazol-3-yl)phthalazin-1(2*H*)-one – 1{36,35,1}



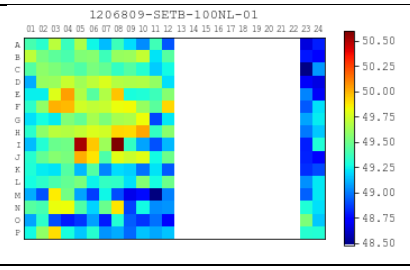
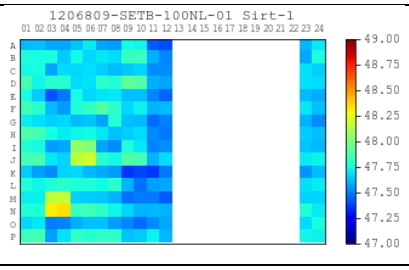
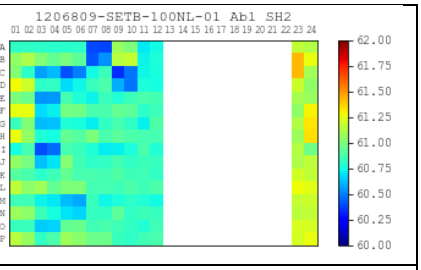
Yield: 20% (42 mg)
LC/MS (APSI) m/z [M+H] calculated for Chemical Formula: $C_{26}H_{35}N_7O_2$: 478.3, found: 478.2.

2-((4-(1-(benzo[*d*][1,3]dioxol-5-ylmethyl)-1*H*-tetrazol-5-yl)piperazin-1-yl)methyl)quinazolin-4(3*H*)-one – 2{1,1}



Yield: 55% (117 mg)
LC/MS (APSI) m/z [M+H] calculated for Chemical Formula: $C_{22}H_{22}N_8O_3$: 447.2, found: 447.

T_m heatmaps on the loaded plates, assays with: a) BRD4, b) SIRT1, c) Abl CH2.

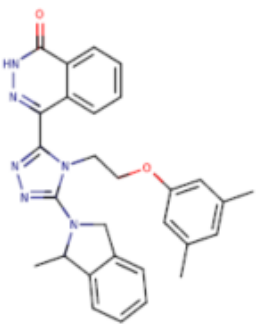
		
a)	b)	c)

Results of the thermal shift assays.

compound	docking score	Well	*dTmD in assays:*		
			Abl SH2	**BrD4**	**SIRT1**
1{1,1,1}	-44.26	C09	-0.64	0.32	0.07
1{2,2,1}	-43.78	A05	-0.25	0.32	-0.02
1{3,3,2}	-43.48	C07	-0.28	0.35	0.01
1{4,4,1}	-43.44	I09	-0.33	0.31	0.11
1{5,5,1}	-42.99	K07	-0.25	0.04	-0.05
1{7,7,4}	-42.54	E09	-0.23	0.22	-0.06
1{8,8,1}	-42.05	E07	-0.26	0.54	0.04
1{9,9,1}	-41.75	G09	-0.24	0.64	-0.07
1{10,10,1}	-41.74	G05	-0.28	0.45	-0.03
1{12,12,1}	-41.67	E07	-0.26	0.54	0.04
1{13,13,6}	-41.58	E03	-0.5	0.76	-0.19
1{16,9,8}	-41.16	A09	-0.01	0.18	0.08
1{17,17,1}	-41.1	C05	-0.53	0.35	-0.02
1{19,19,9}	-40.91	K05	-0.15	0.11	0.01
1{20,20,1}	-40.89	O07	-0.2	-0.15	0
1{21,21,9}	-40.61	E05	-0.21	0.46	0.05
1{22,22,1}	-40.54	I07	-0.32	0.48	-0.05
1{23,23,1}	-40.52	M05	-0.47	-0.1	0.03
1{24,24,10}	-40.48	A07	-0.71	0.14	-0.09
1{25,24,11}	-40.47	I03	-0.57	0.29	-0.09
1{26,25,12}	-40.41	G03	-0.43	0.38	-0.02
1{28,27,1}	-40.27	O03	-0.37	-0.14	-0.18
1{29,28,4}	-40.23	O05	-0.12	-0.11	0
1{30,29,14}	-40.19	C03	-0.41	0.35	0.02
1{31,30,9}	-40.12	A03	-0.25	0.2	-0.09
1{32,31,15}	-40.04	I05	-0.26	0.75	0.39
1{35,34,16}	-39.95	M03	-0.37	0.6	0.53
1{36,35,1}	-39.91	M07	-0.29	0.14	-0.02
2{1,1}	-39.69	K03	-0.23	0.19	0.01

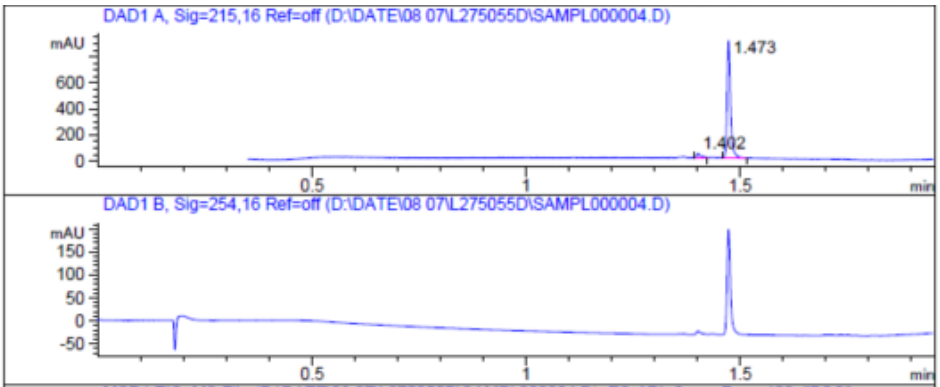
Spectral data for the synthesized compounds.

LC/MS spectrum of 1{1,1,1}

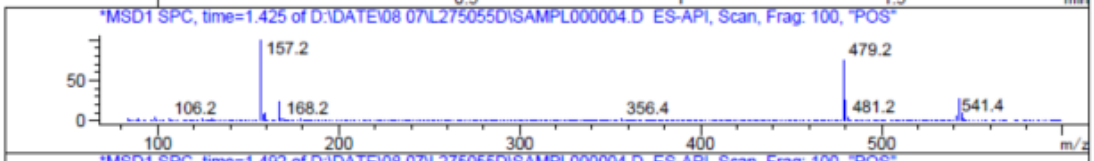


Mol Wt 492.57
Exact Mass 492.26

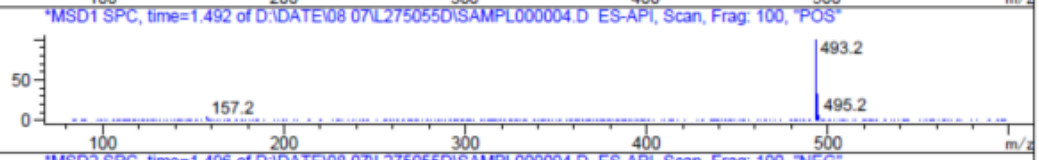
#	Time	Area%
1	1.402	4.90
2	1.473	95.10



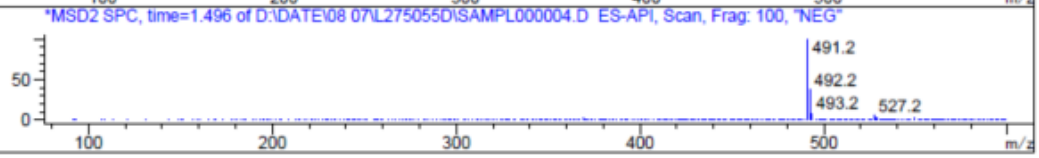
RT 1.425



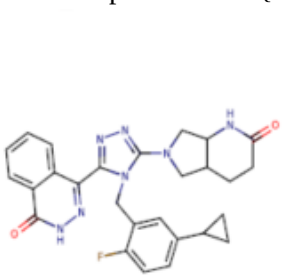
RT 1.494



RT 1.494



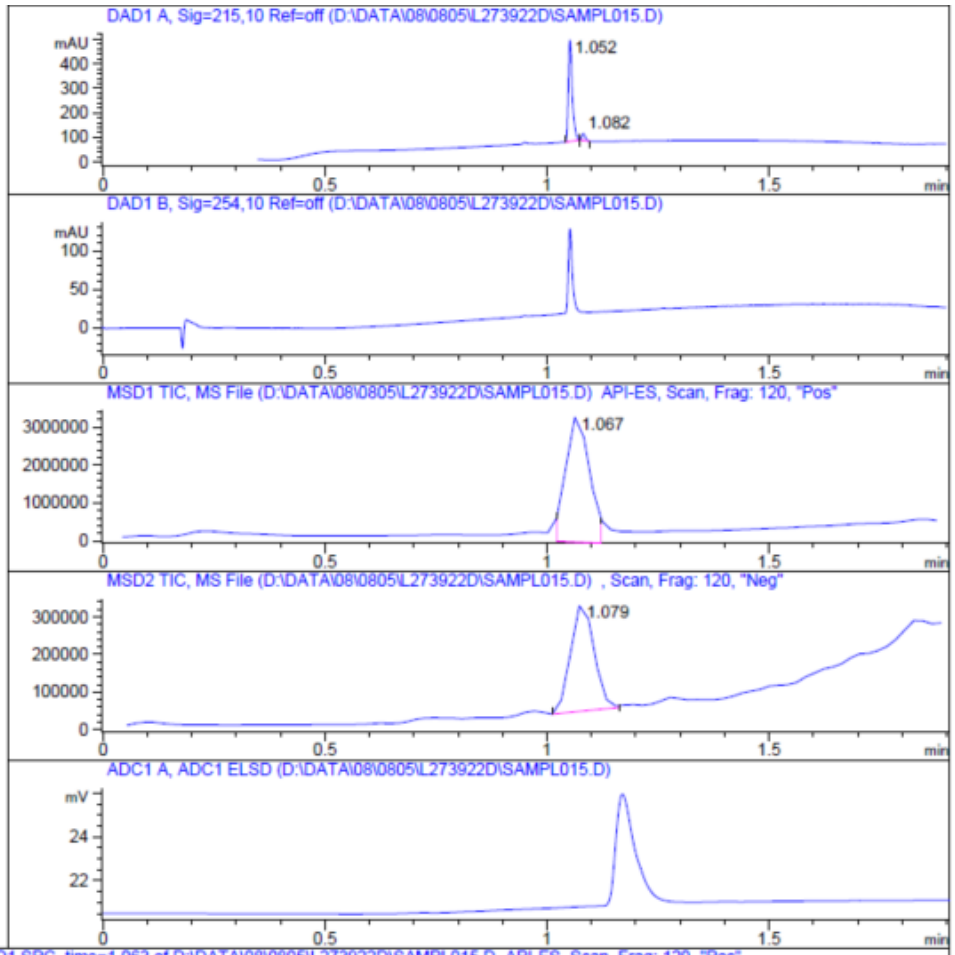
LC/MS spectrum of 1{2,2,1}



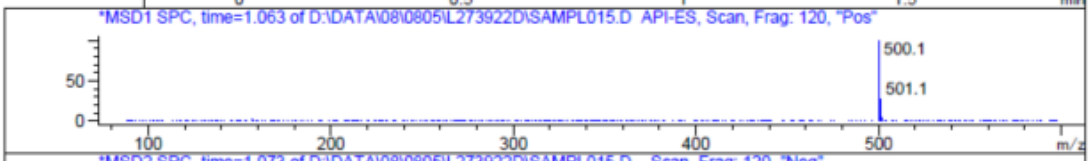
Mol Wt **499.54**

Exact Mass **499.24**

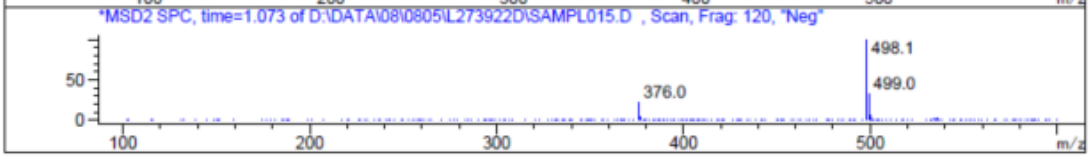
#	Time	Area%
1	1.052	94.42
2	1.082	5.58



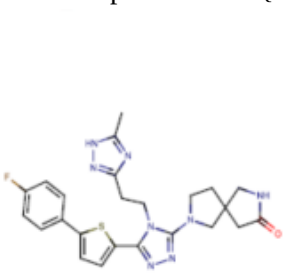
RT 1.067



RT 1.079



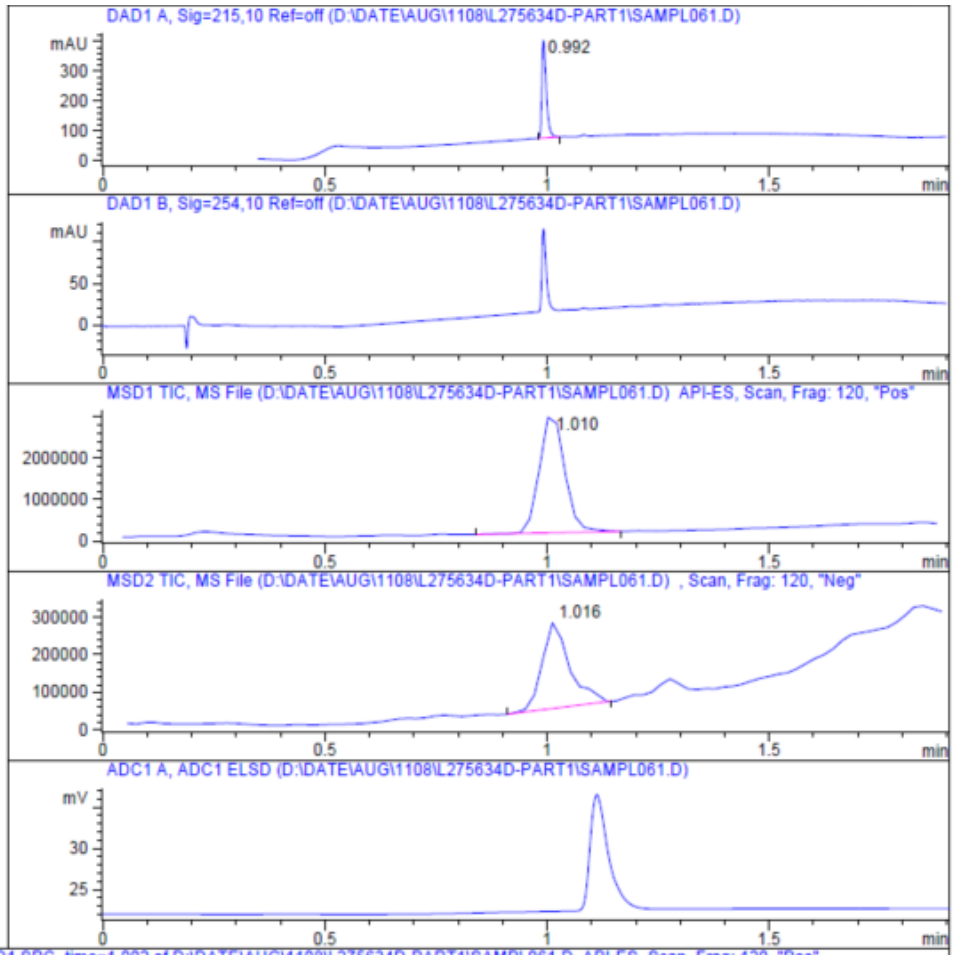
LC/MS spectrum of 1{3,3,2}



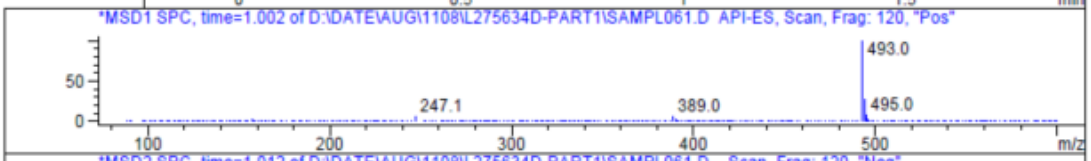
Mol Wt **492.57**

Exact Mass **492.21**

#	Time	Area%
1	0.992	100.00

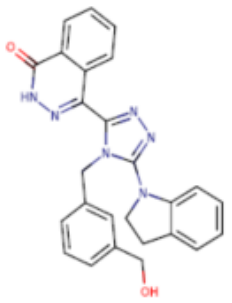


RT 1.010



RT 1.016

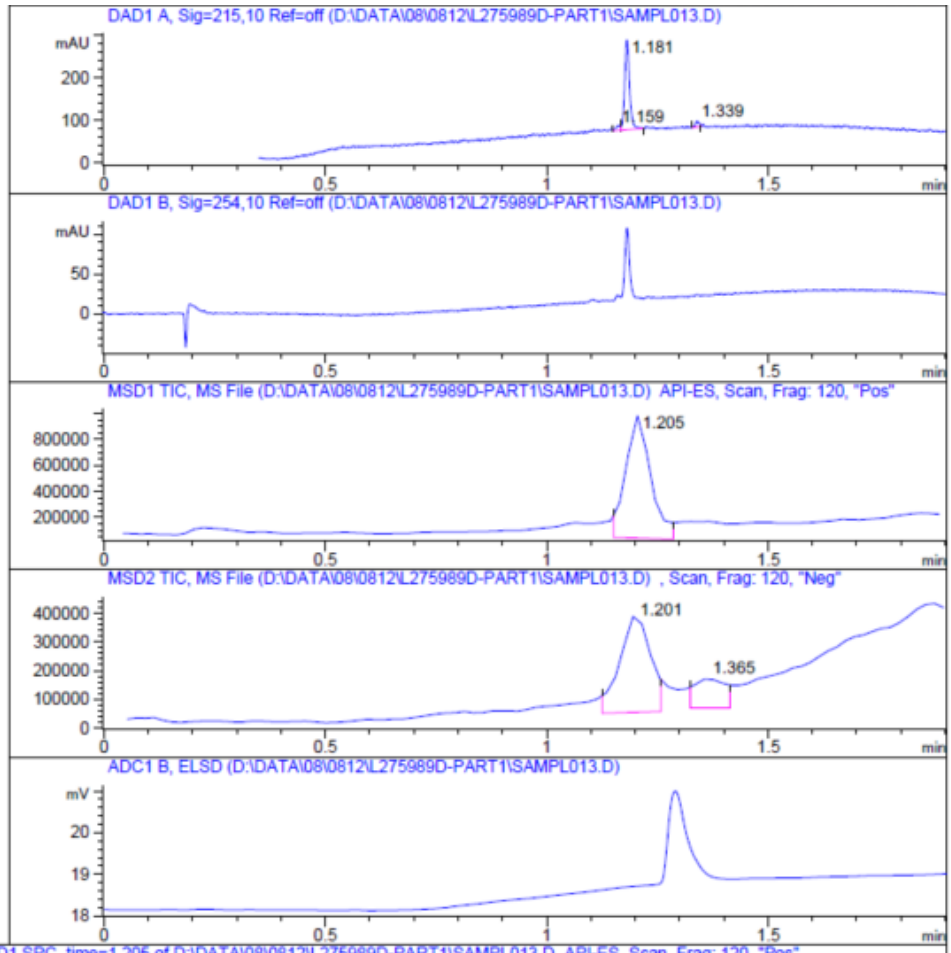
LC/MS spectrum of 1{4,4,1}



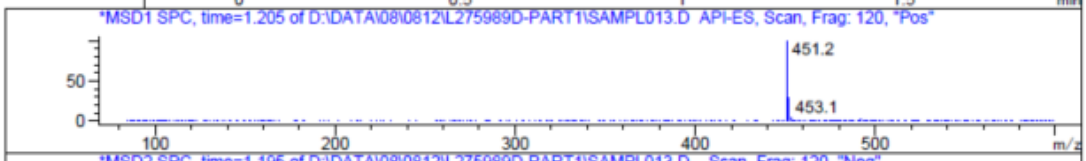
Mol Wt **450.49**

Exact Mass **450.2**

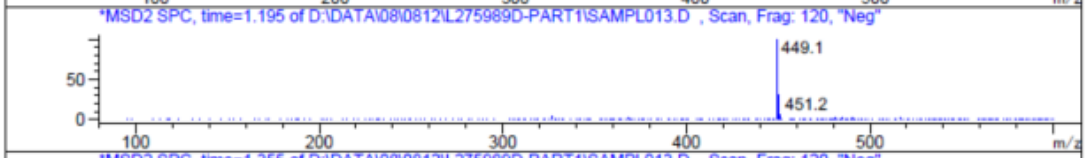
#	Time	Area%
1	1.159	4.59
2	1.181	90.90
3	1.339	4.50



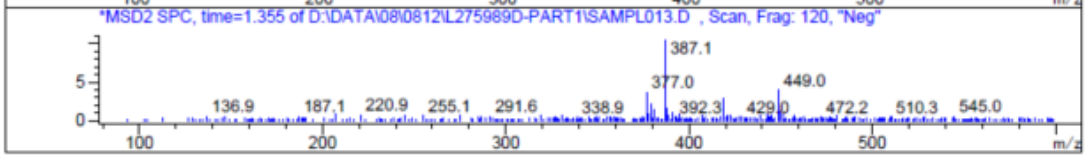
RT 1.205



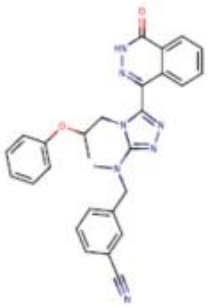
RT 1.201



RT 1.365



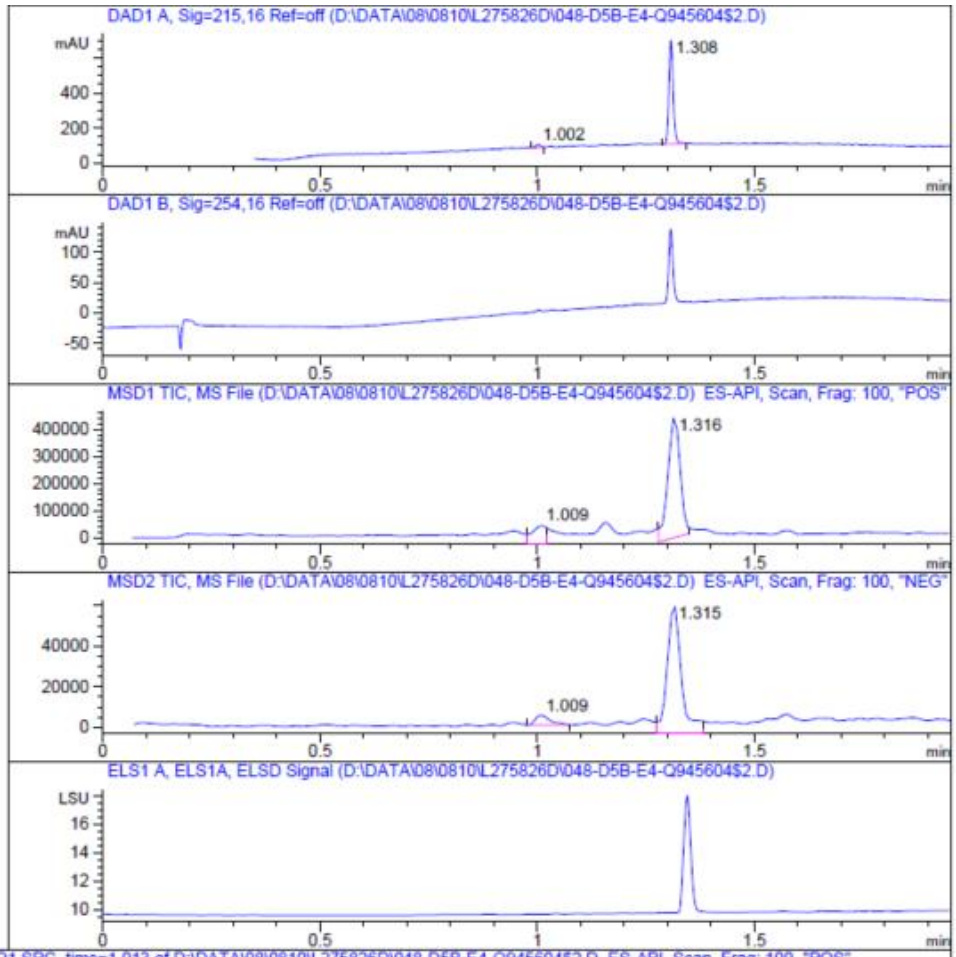
LC/MS spectrum of 1{5,5,1}



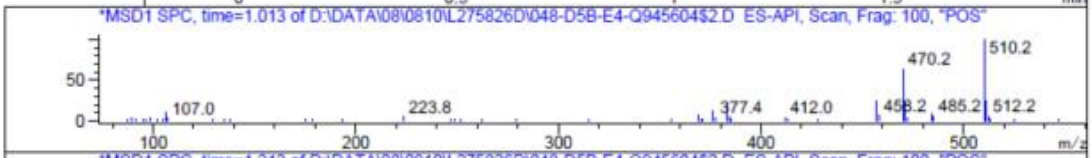
Mol Wt **491.54**

Exact Mass **491.23**

#	Time	Area%
1	1.002	3.38
2	1.308	96.62

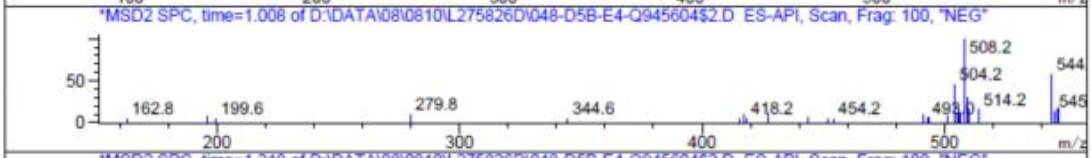


RT 1.009

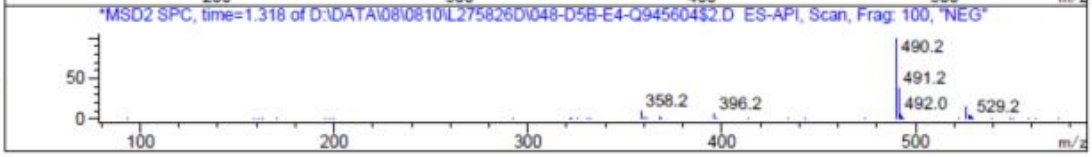


RT 1.316

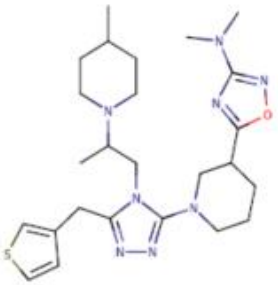
RT 1.009



RT 1.315



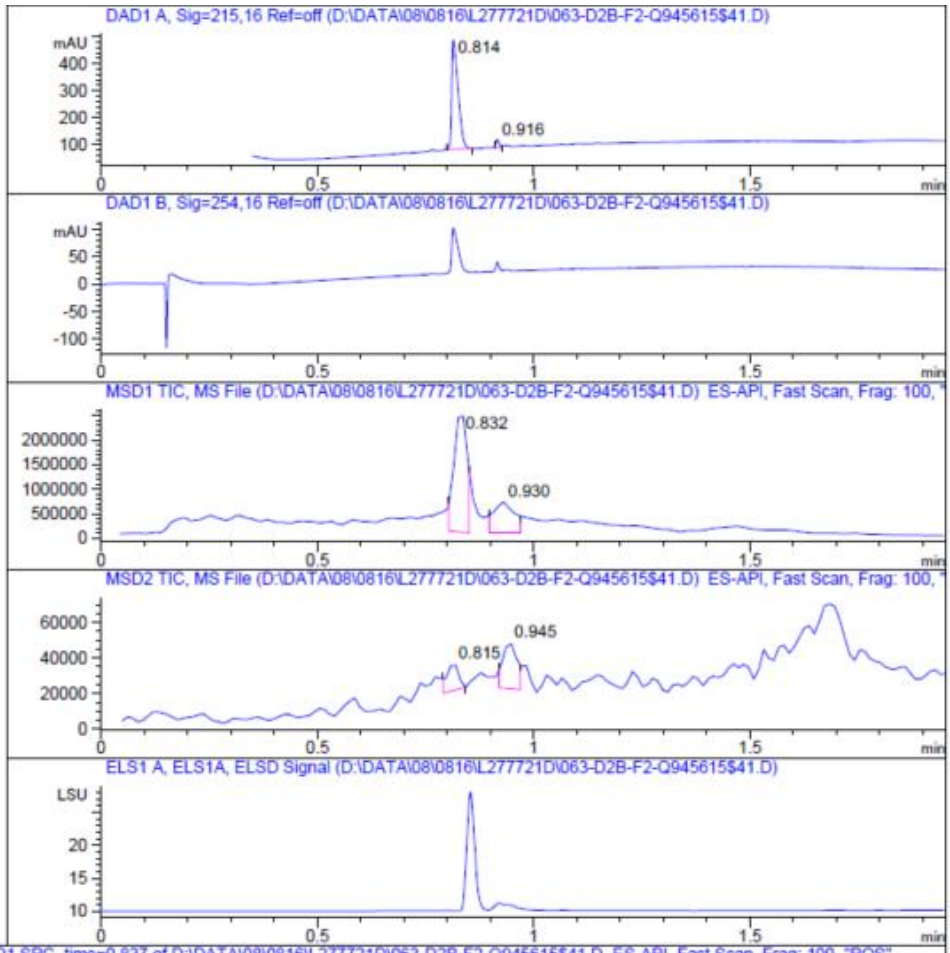
LC/MS spectrum of 1{7,7,4}



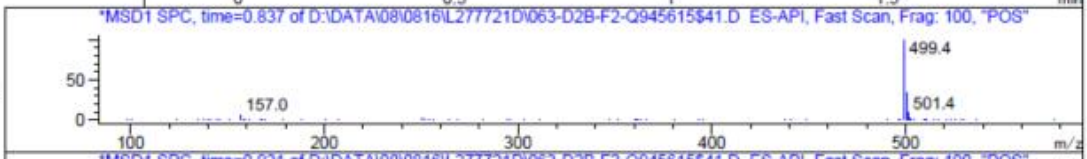
Mol Wt 498.69

Exact Mass 498.34

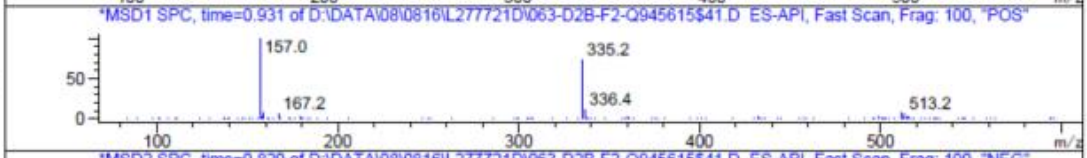
#	Time	Area%
1	0.814	96.19
2	0.916	3.81



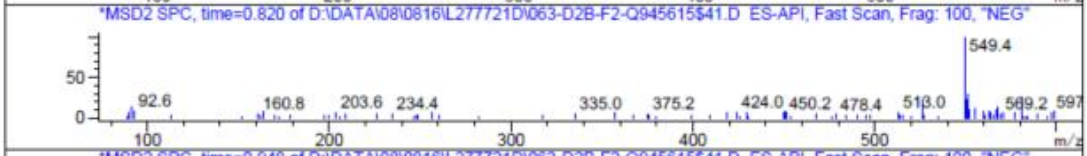
RT 0.832



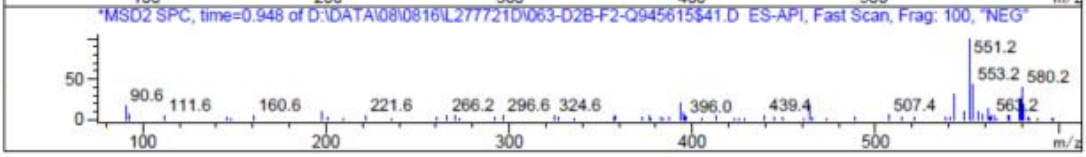
RT 0.930



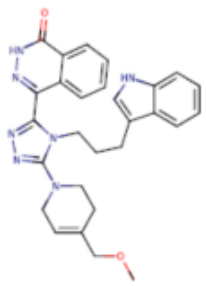
RT 0.815



RT 0.945



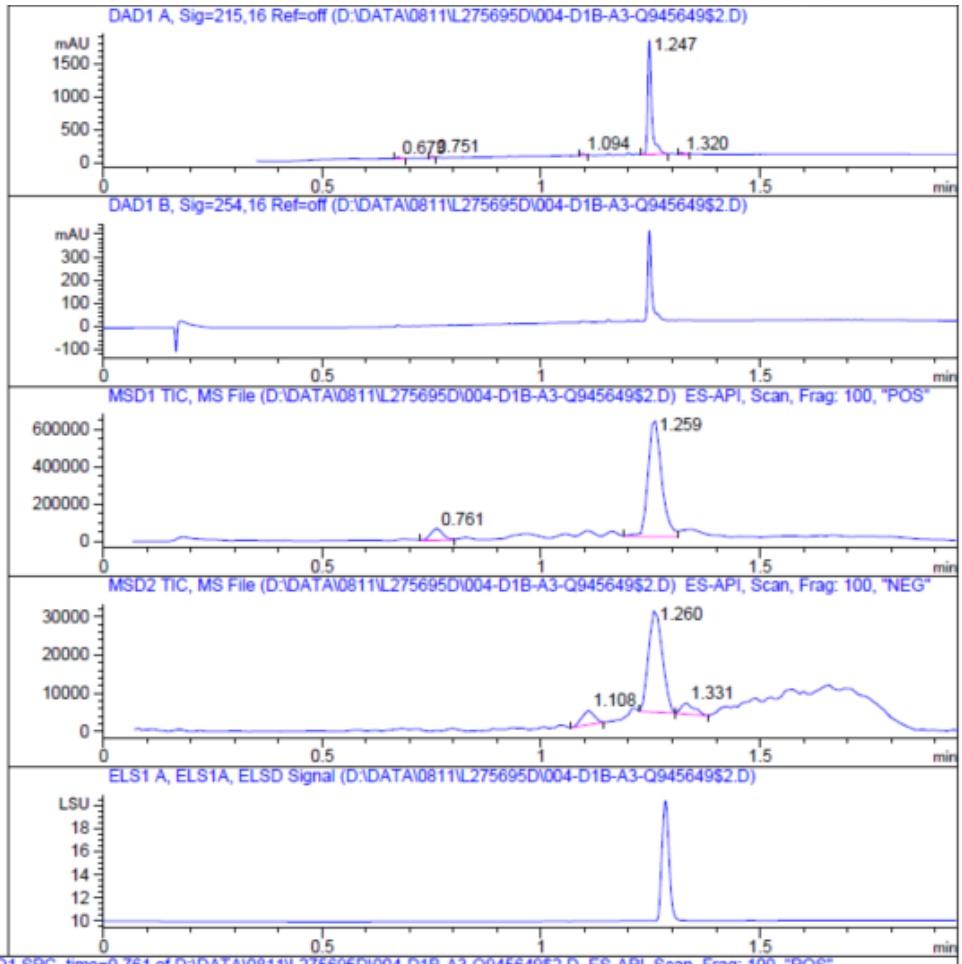
LC/MS spectrum of 1{8,8,1}



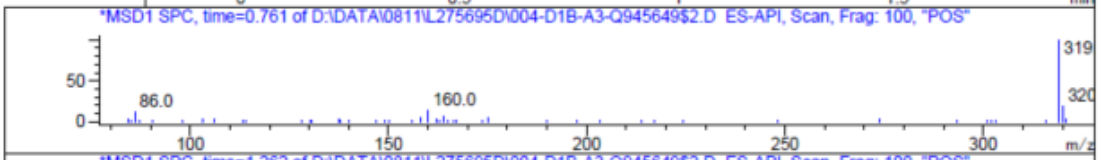
Mol Wt **495.58**

Exact Mass **495.27**

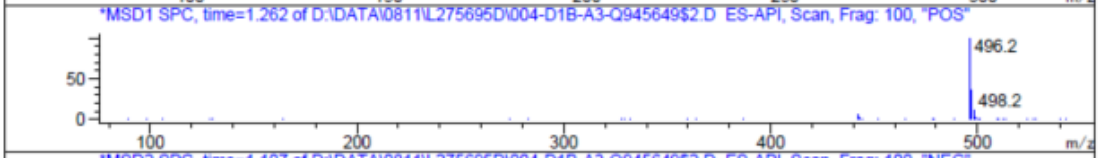
#	Time	Area%
1	0.673	1.08
2	0.751	1.02
3	1.094	1.32
4	1.247	95.37
5	1.320	1.21



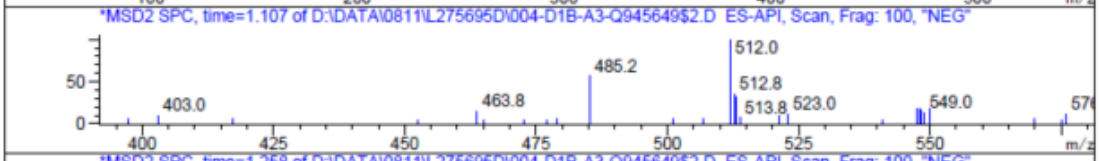
RT 0.761



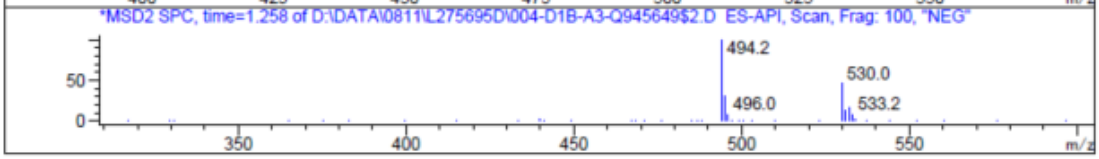
RT 1.259



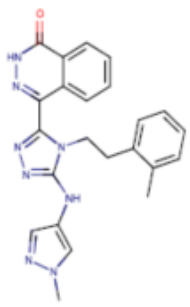
RT 1.108



RT 1.260



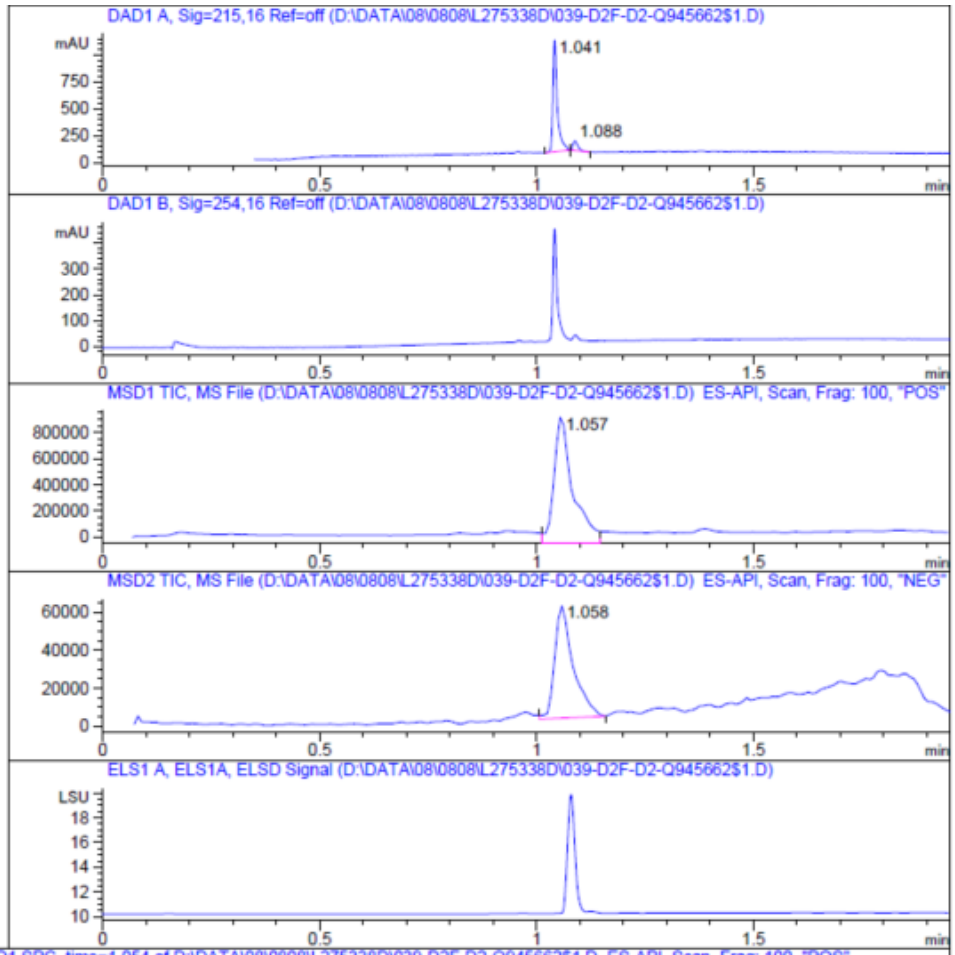
LC/MS spectrum of 1{9,9,1}



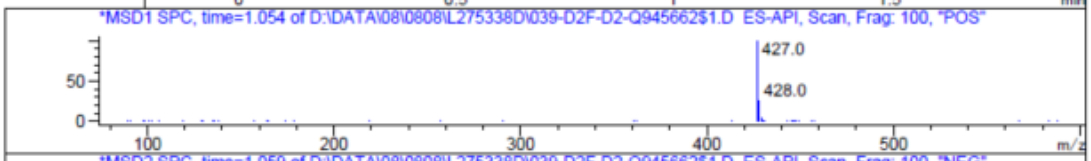
Mol Wt **426.47**

Exact Mass **426.21**

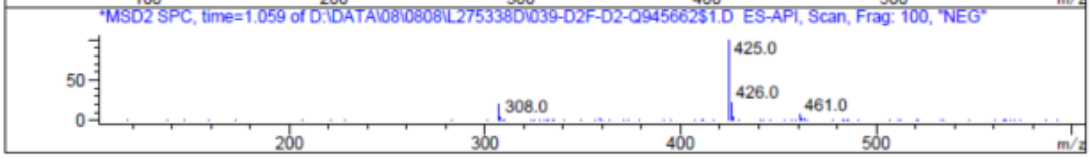
#	Time	Area%
1	1.041	91.27
2	1.088	8.73



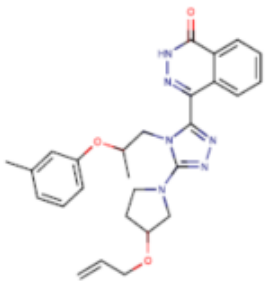
RT 1.057



RT 1.058



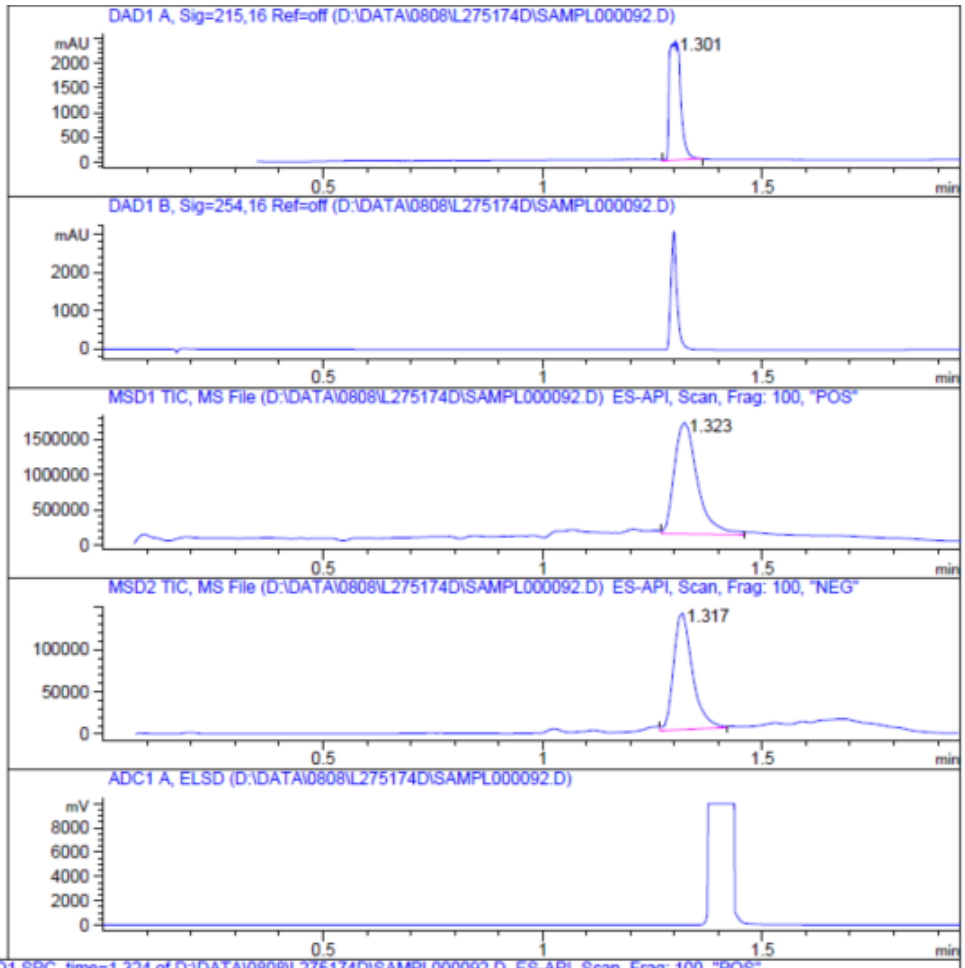
LC/MS spectrum of 1{10,10,1}



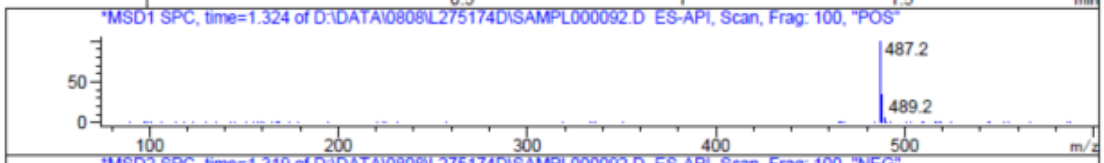
Mol Wt **486.57**

Exact Mass **486.27**

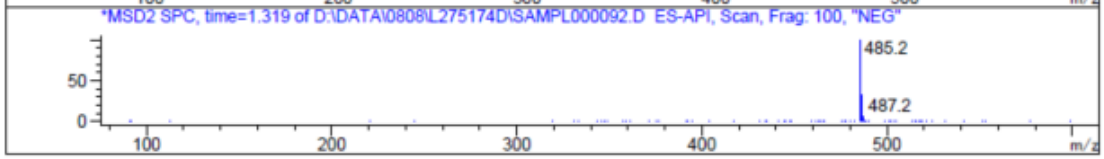
#	Time	Area%
1	1.301	100.00



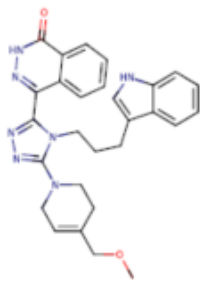
RT 1.323



RT 1.317



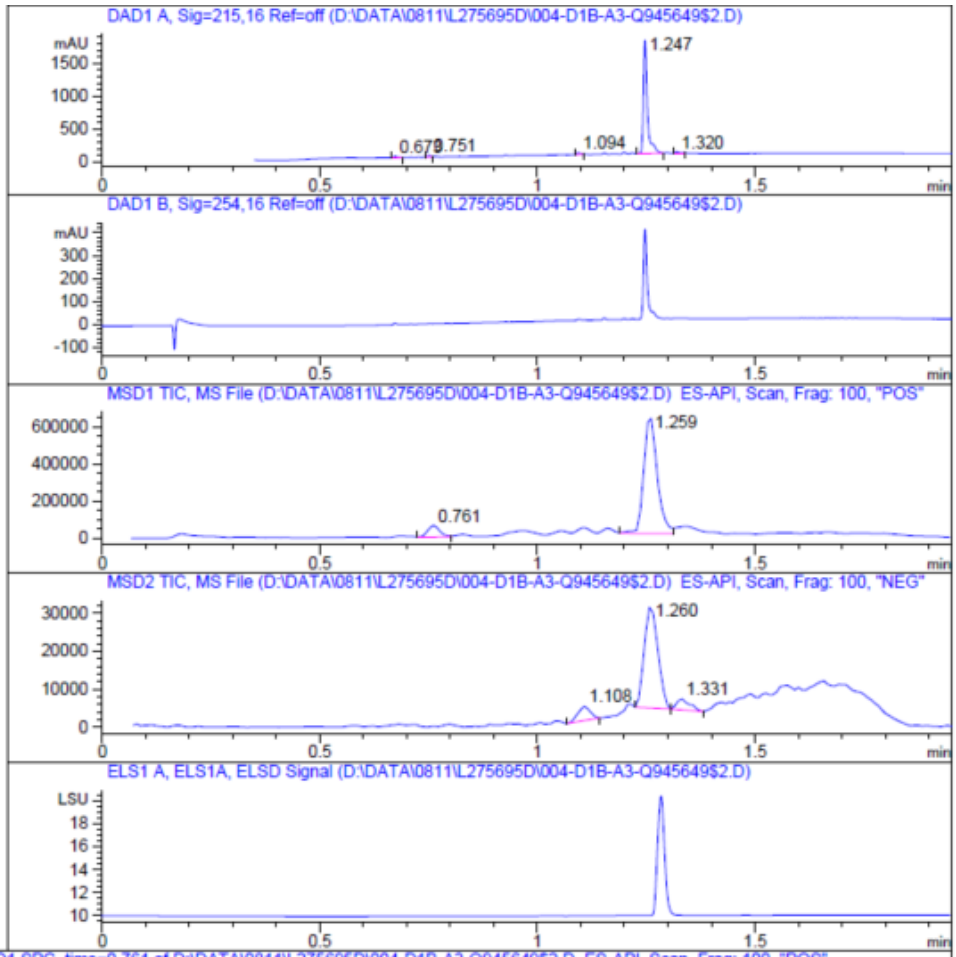
LC/MS spectrum of 1{12,12,1}

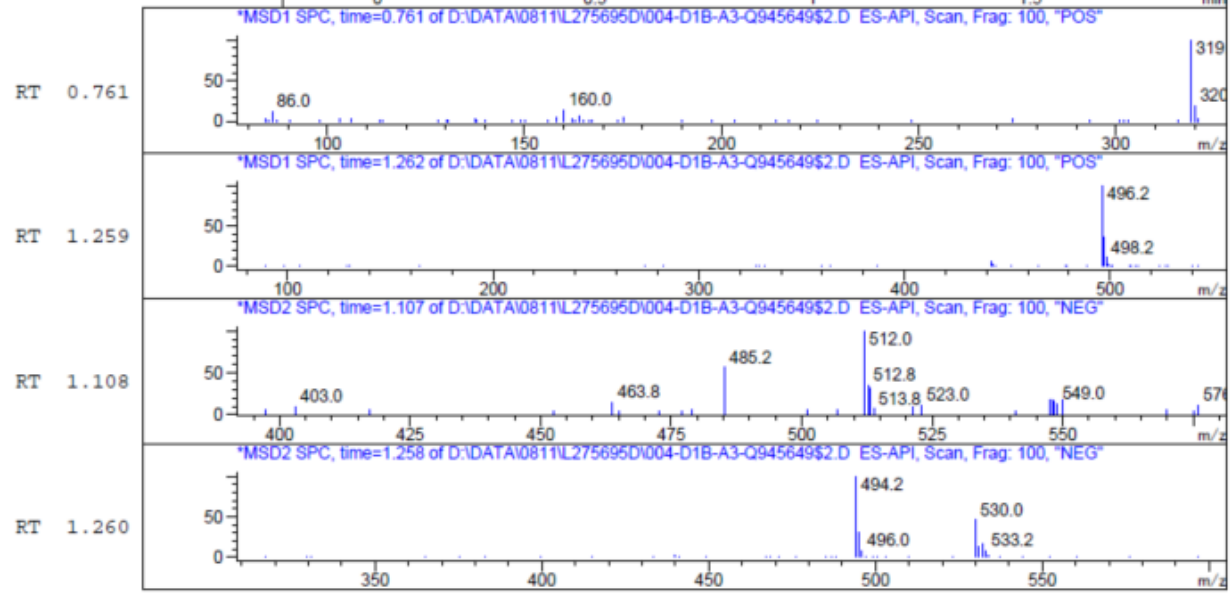


Mol Wt **495.58**

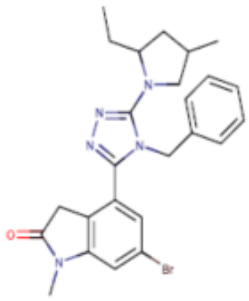
Exact Mass **495.27**

#	Time	Area%
1	0.673	1.08
2	0.751	1.02
3	1.094	1.32
4	1.247	95.37
5	1.320	1.21





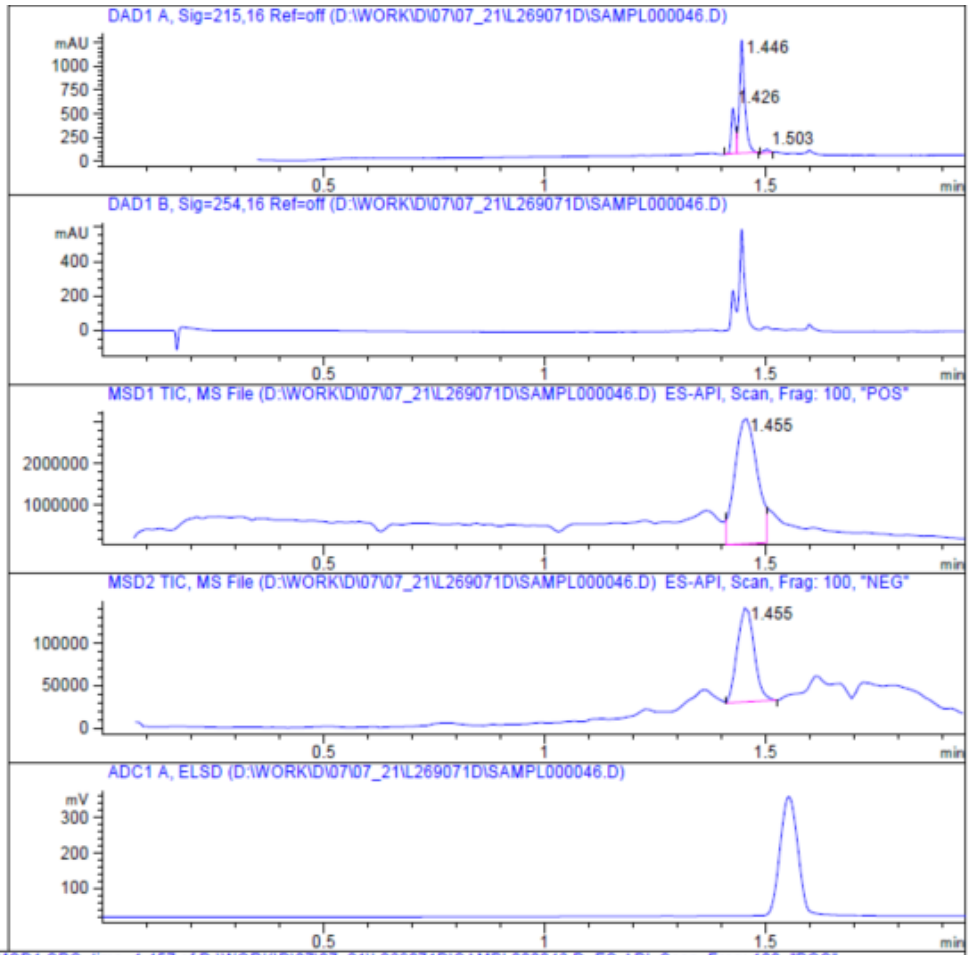
LC/MS spectrum of 1{13,13,6}



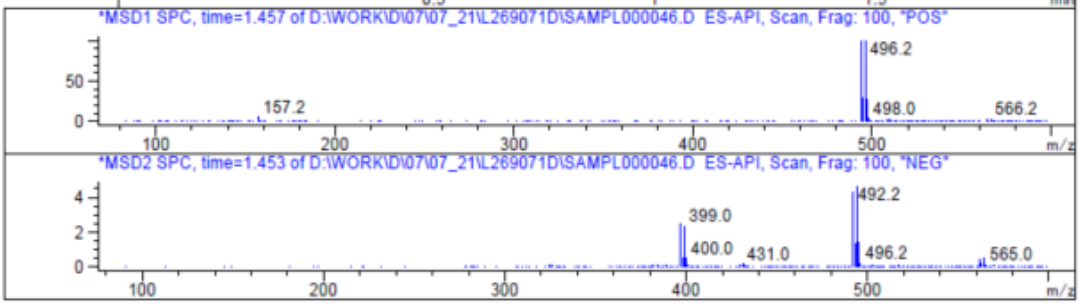
Mol Wt **494.43**

Exact Mass **495.19**

#	Time	Area%
1	1.426	22.74
2	1.446	74.89
3	1.503	2.37

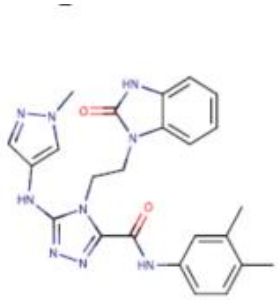


RT 1.455



RT 1.455

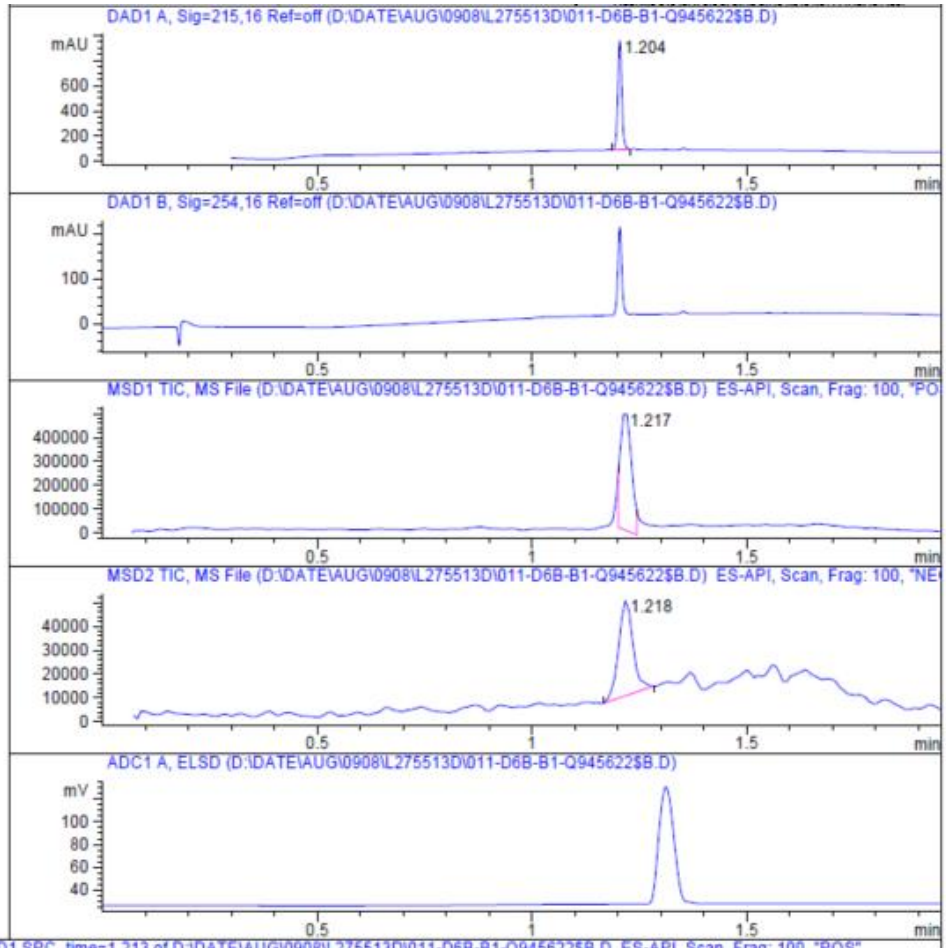
LC/MS spectrum of 1{16,9,8}

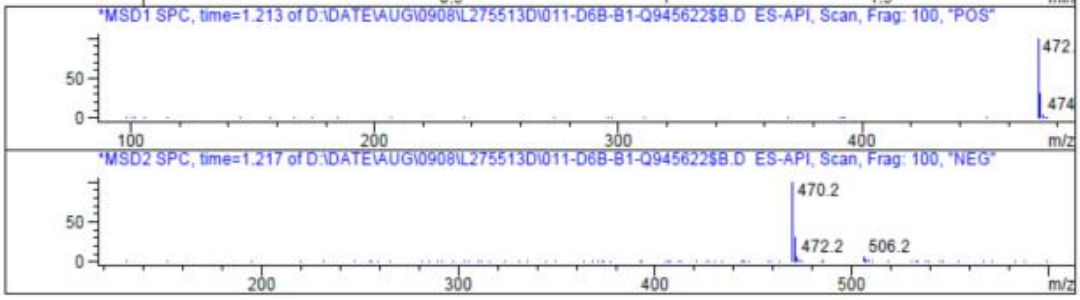


Mol Wt **471.51**

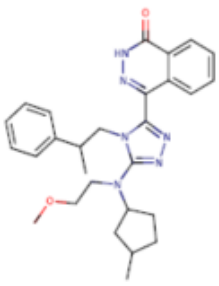
Exact Mass **471.23**

#	Time	Area%
1	1.204	100.00





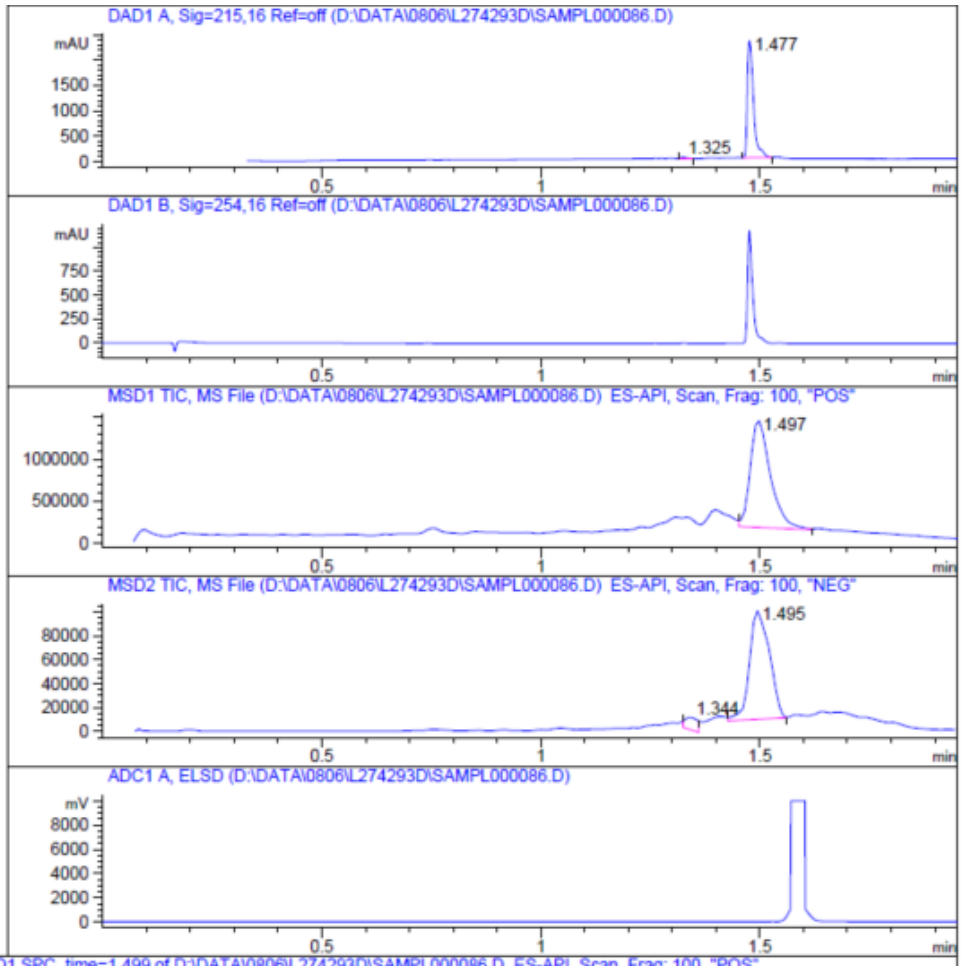
LC/MS spectrum of 1{17,17,1}

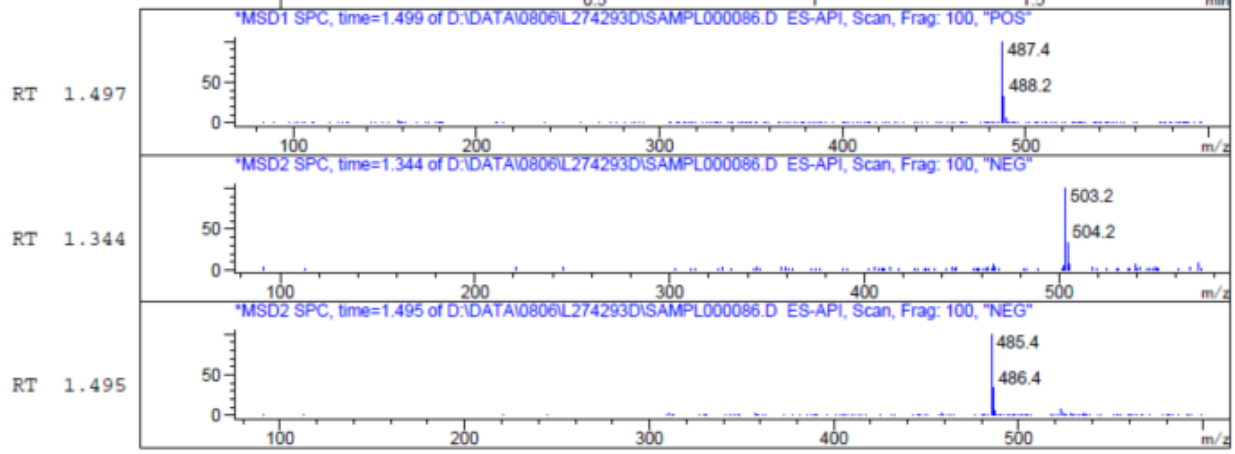


Mol Wt **486.61**

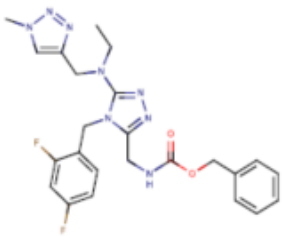
Exact Mass **486.32**

#	Time	Area%
1	1.325	1.04
2	1.477	98.96





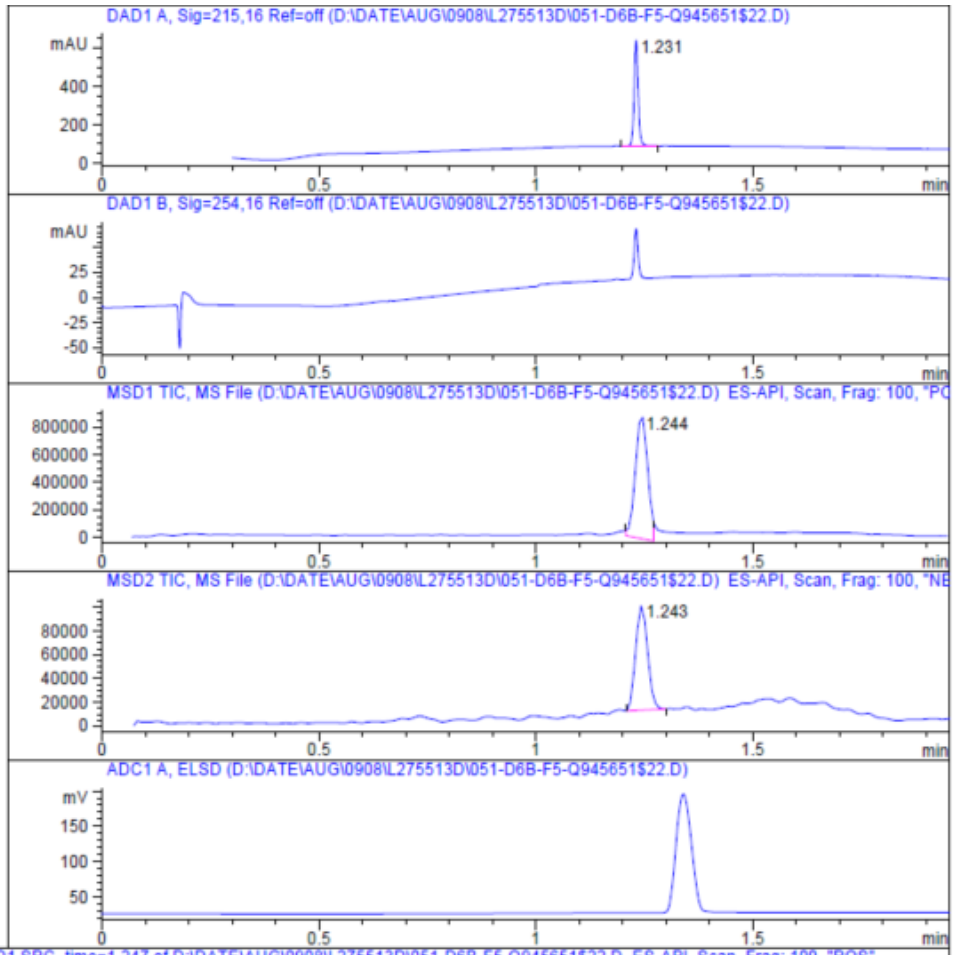
LC/MS spectrum of 1{19,19,9}



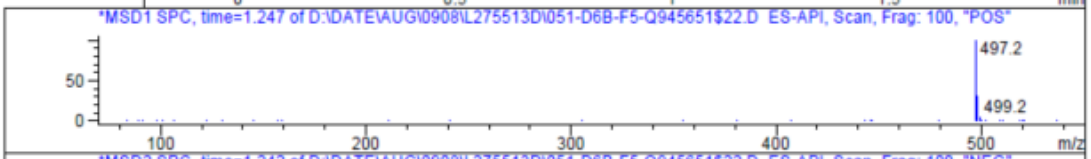
Mol Wt **496.51**

Exact Mass **496.24**

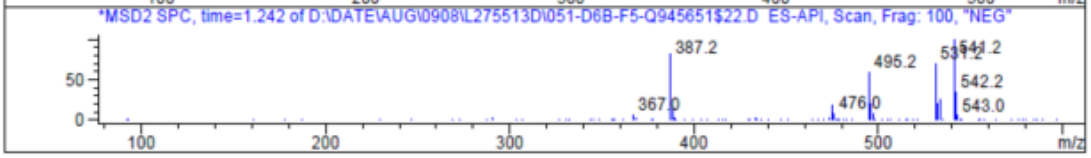
#	Time	Area%
1	1.231	100.00



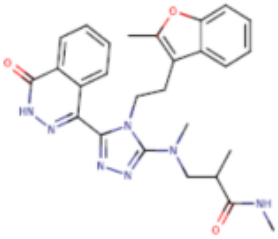
RT 1.244



RT 1.243



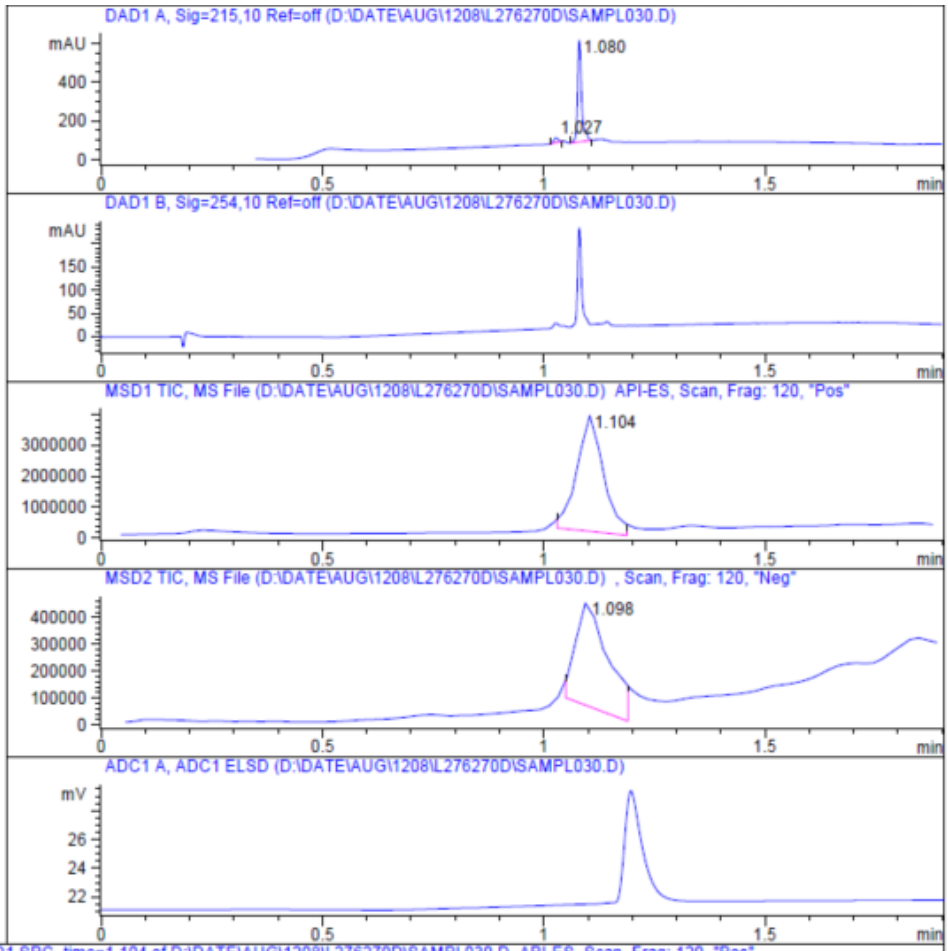
LC/MS spectrum of 1{20,20,1}



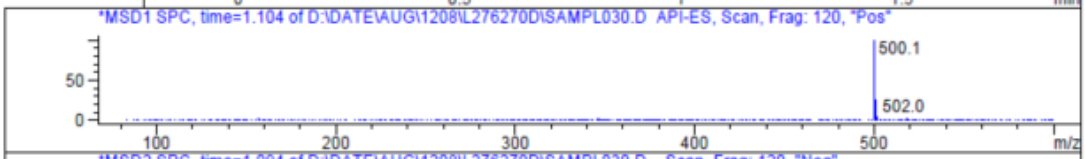
Mol Wt **499.56**

Exact Mass **499.26**

#	Time	Area%
1	1.027	4.87
2	1.080	95.13

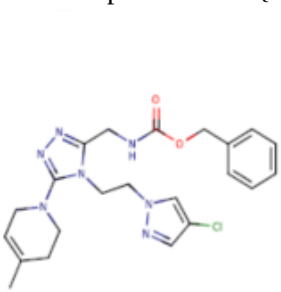


RT 1.104



RT 1.098

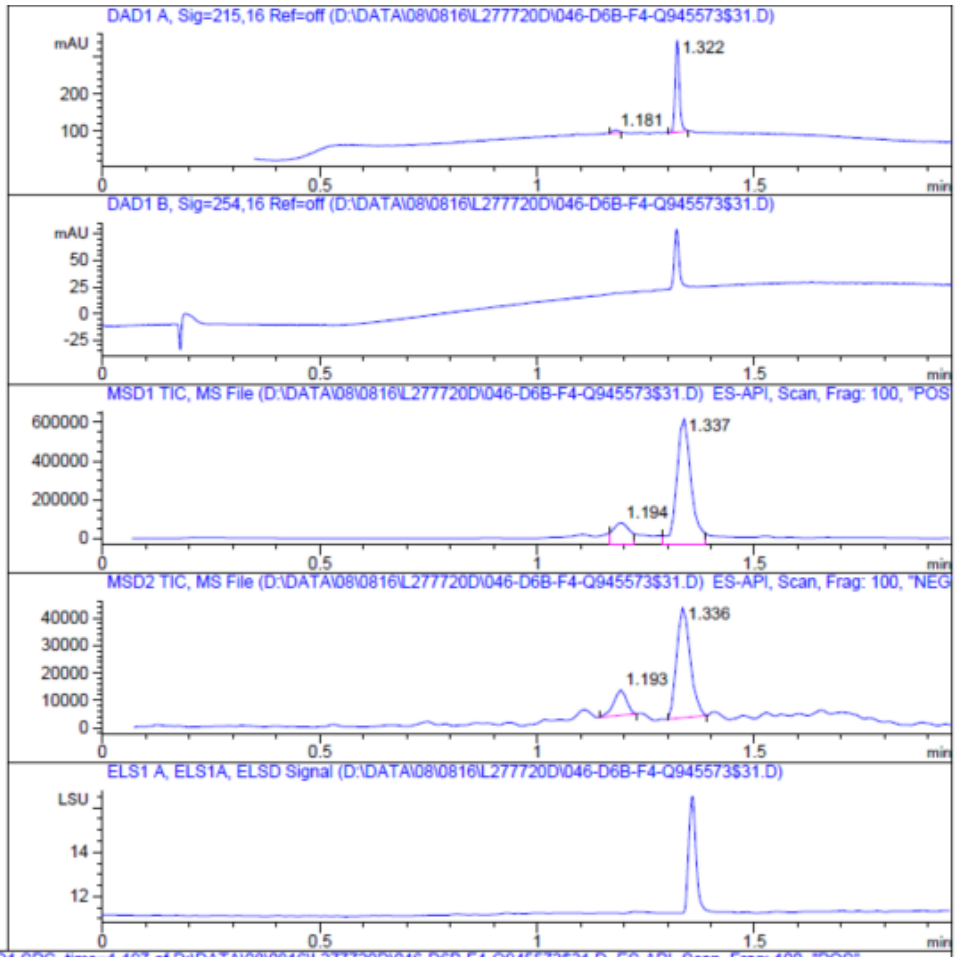
LC/MS spectrum of 1{21,21,9}

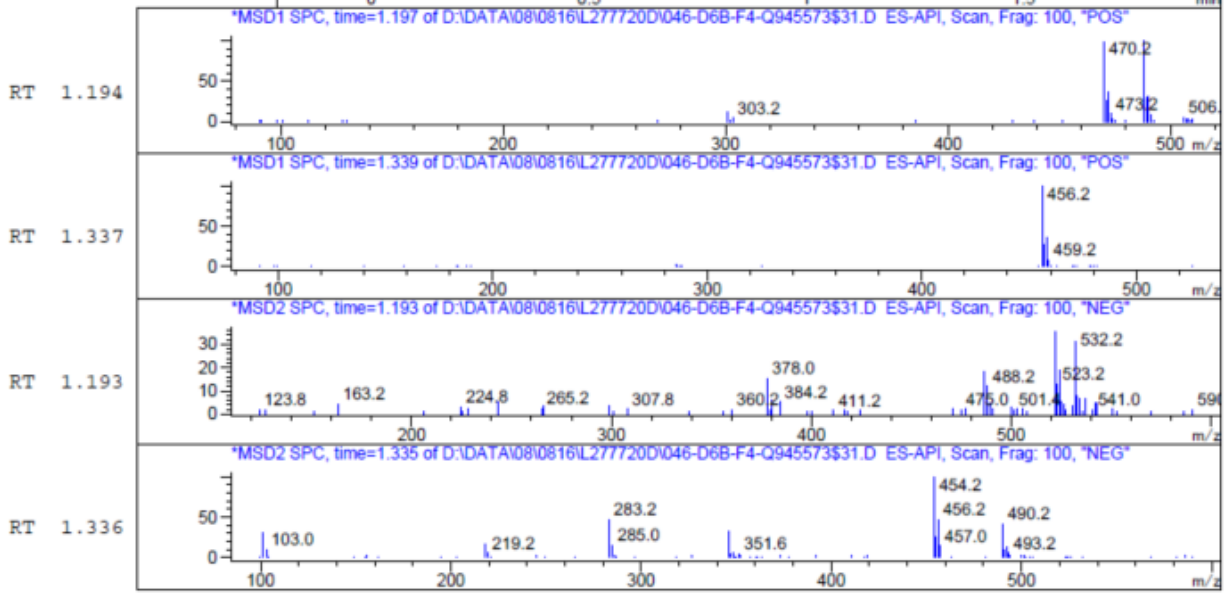


Mol Wt **455.94**

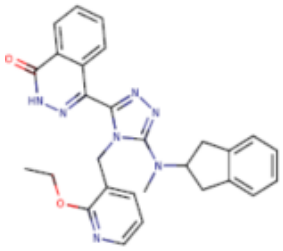
Exact Mass **455.21**

#	Time	Area%
1	1.181	4.66
2	1.322	95.34





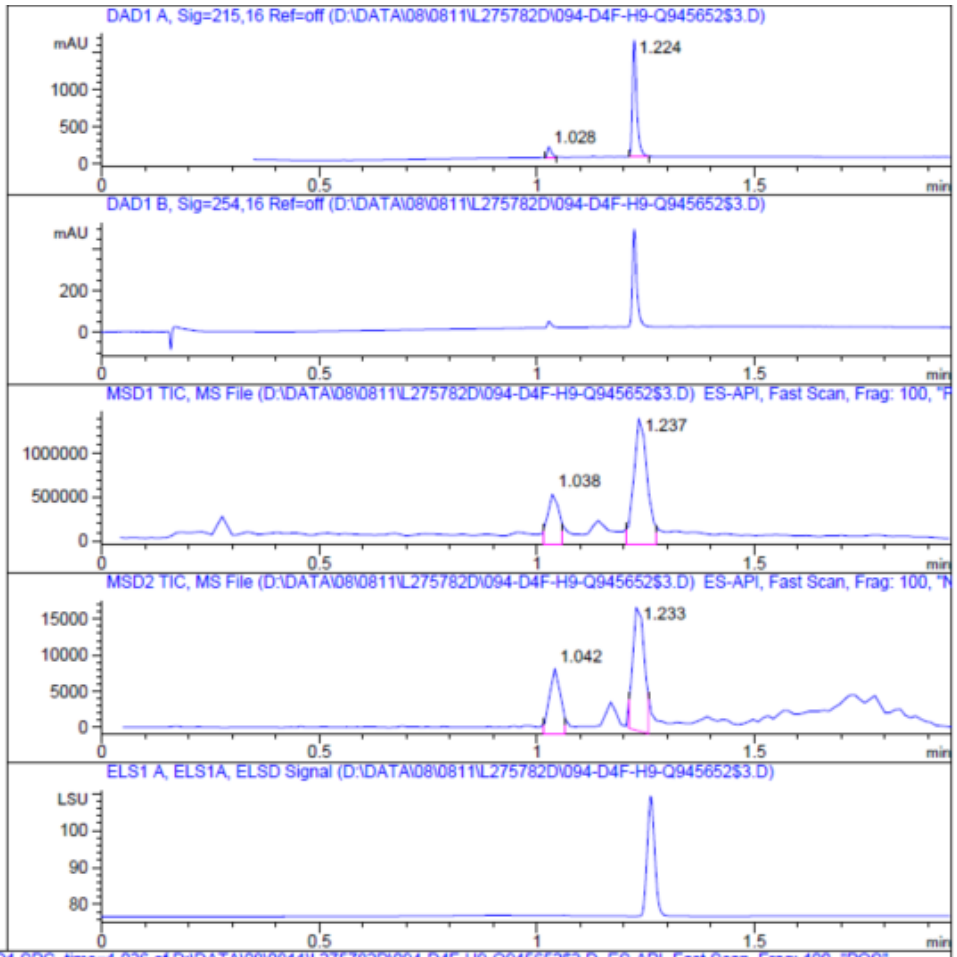
LC/MS spectrum of 1{22,22,1}



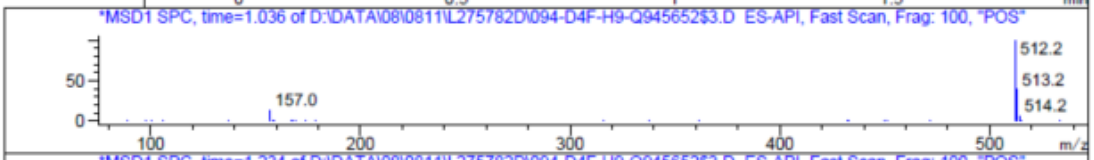
Mol Wt **493.56**

Exact Mass **493.25**

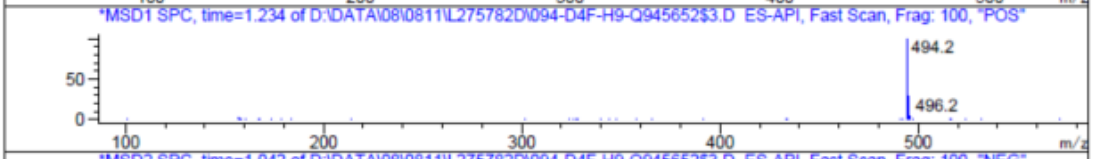
#	Time	Area%
1	1.028	8.31
2	1.224	91.69



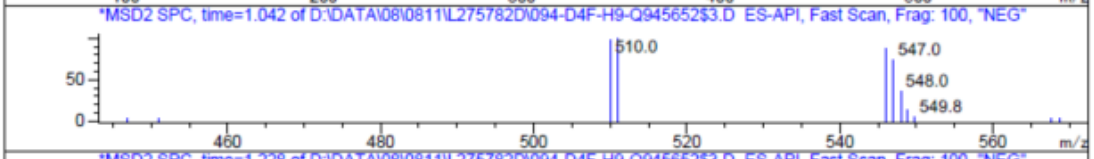
RT 1.038



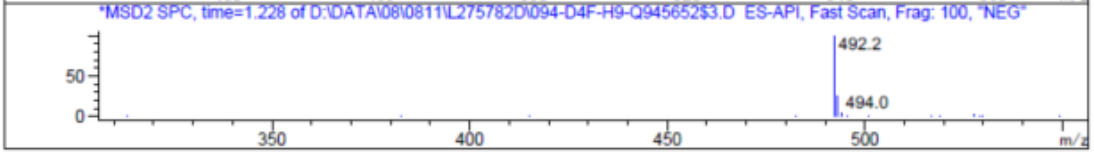
RT 1.237



RT 1.042

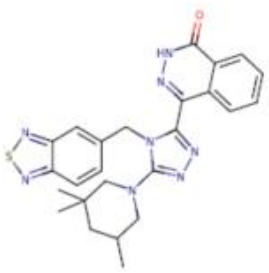


RT 1.233



LC/MS spectrum of 1{23,23,1}

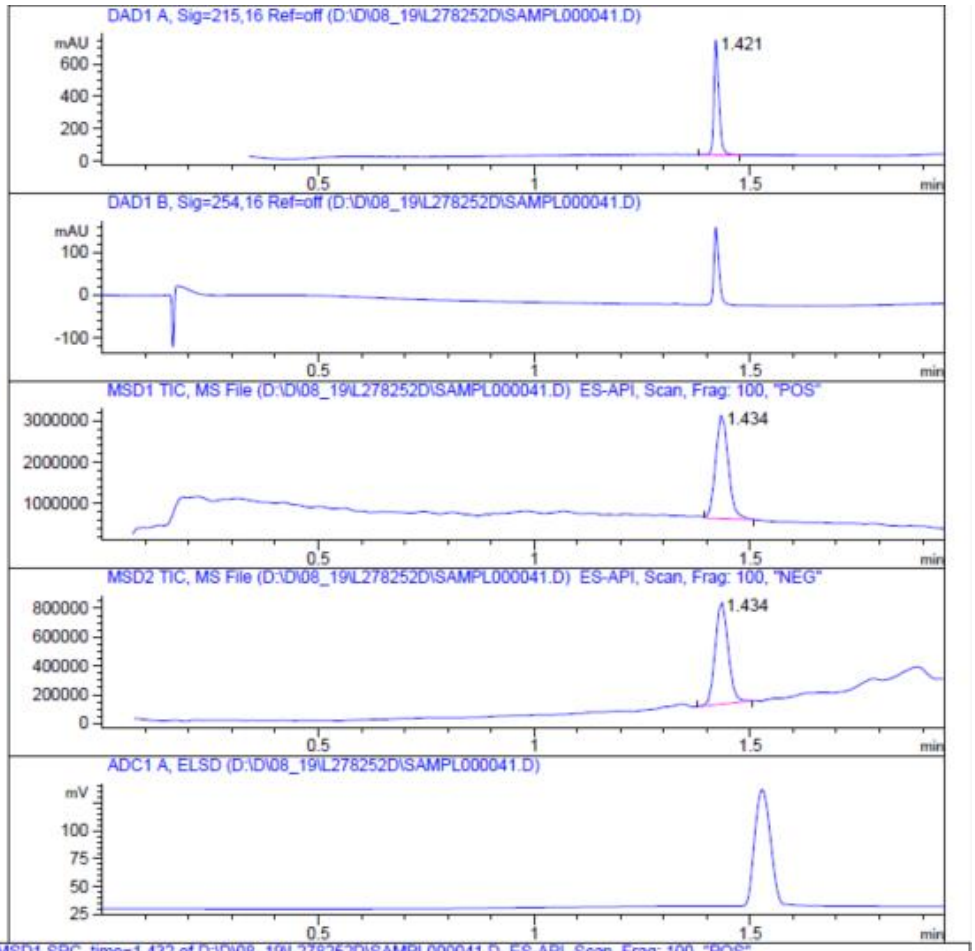
Ret_Time: 1.421 min



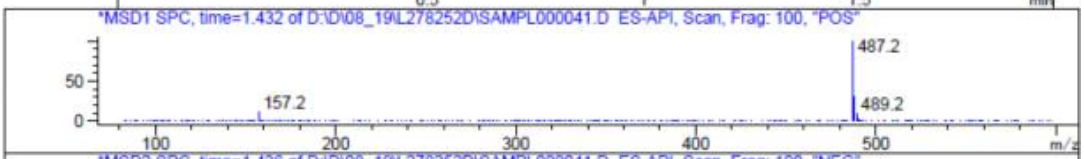
Mol Wt **486.59**

Exact Mass **486.22**

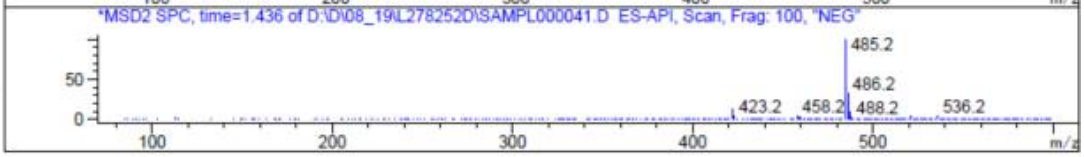
#	Time	Area%
1	1.421	100.00



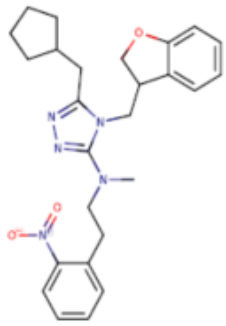
RT 1.434



RT 1.434



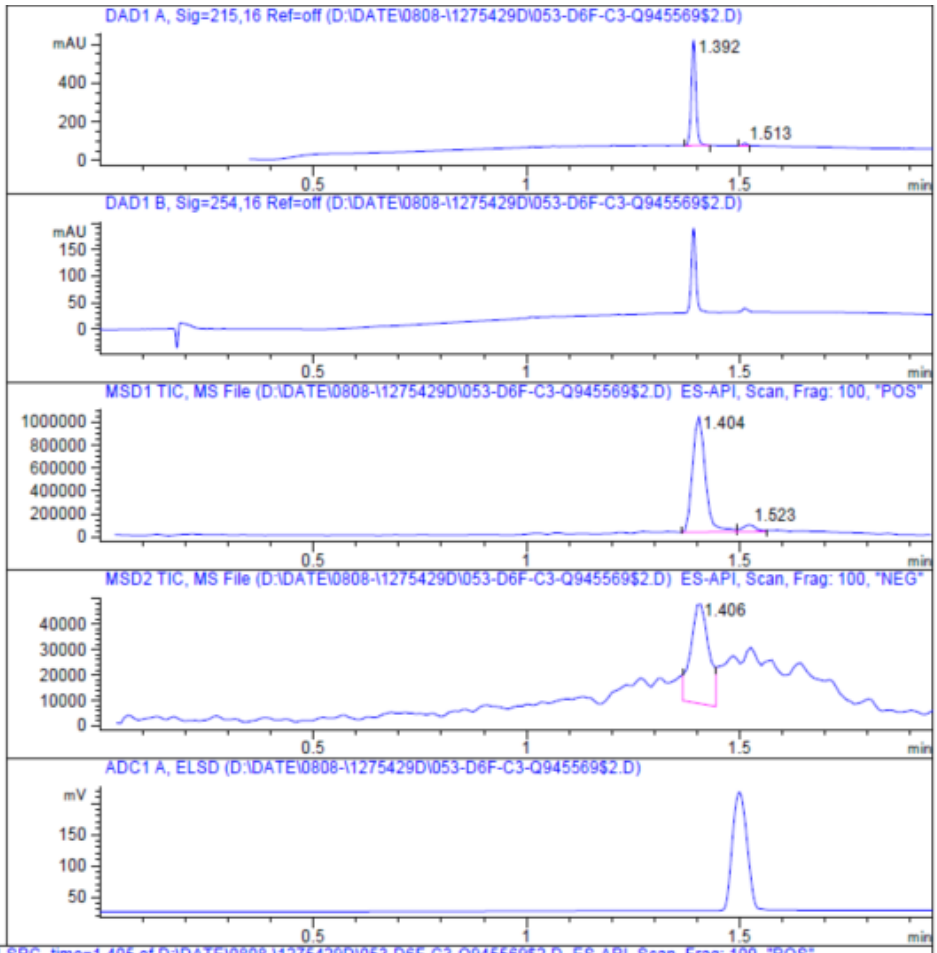
LC/MS spectrum of 1{24,24,10}



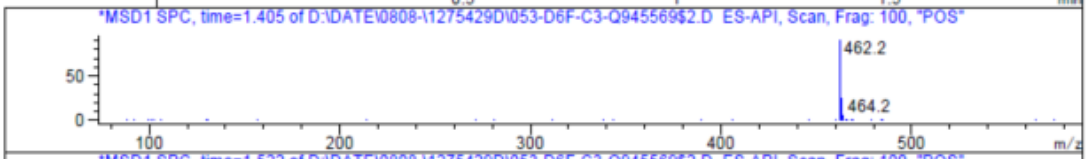
Mol Wt **461.56**

Exact Mass **461.28**

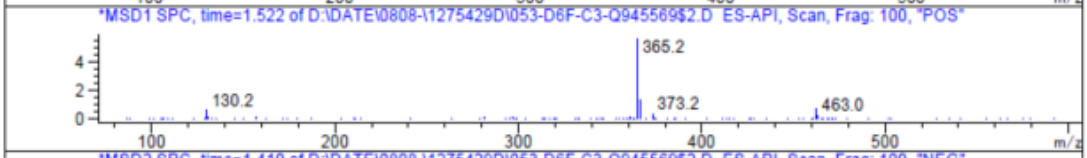
#	Time	Area%
1	1.392	98.04
2	1.513	1.96



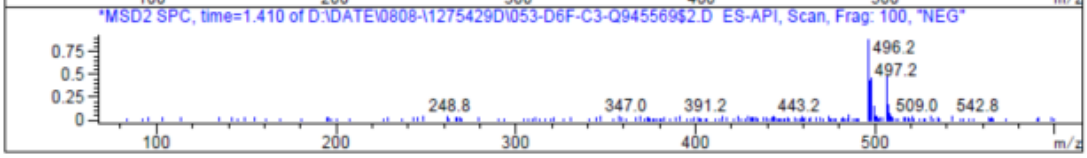
RT 1.404



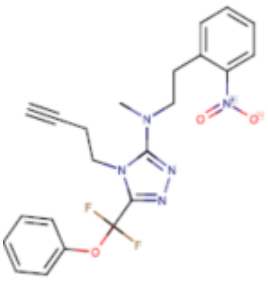
RT 1.523



RT 1.406



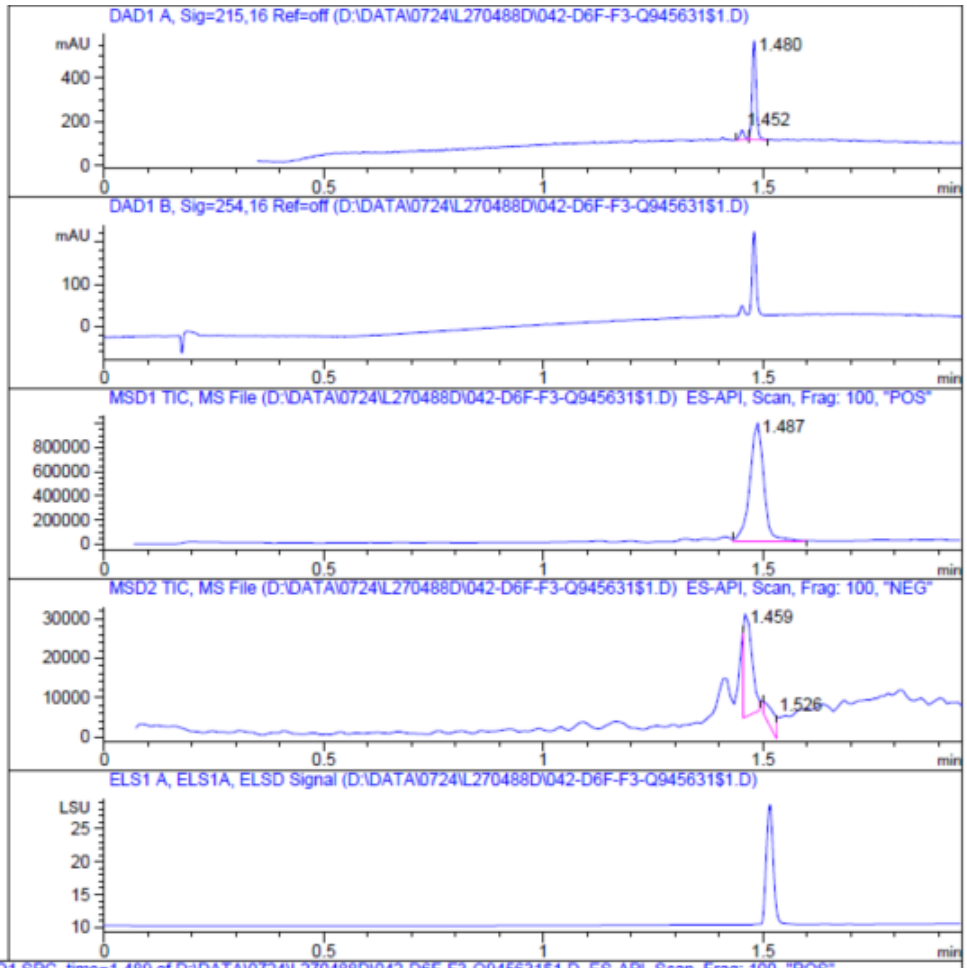
LC/MS spectrum of 1{25,24,11}



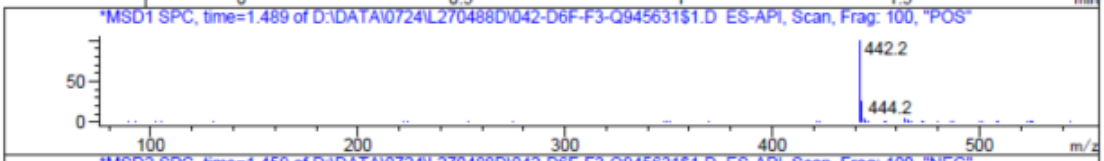
Mol Wt **441.43**

Exact Mass **441.18**

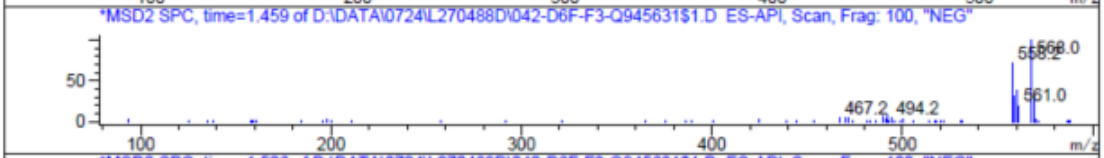
#	Time	Area%
1	1.452	9.81
2	1.480	90.19



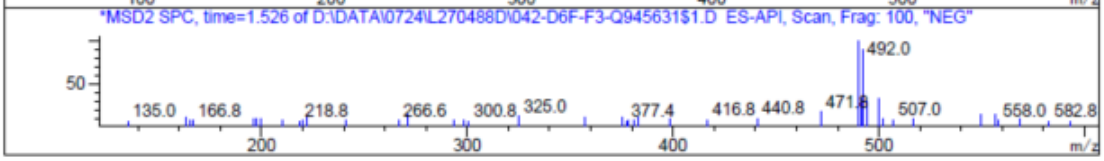
RT 1.487



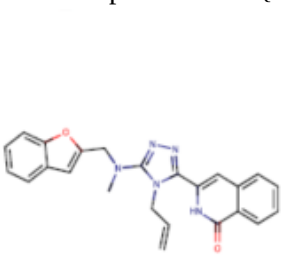
RT 1.459



RT 1.526

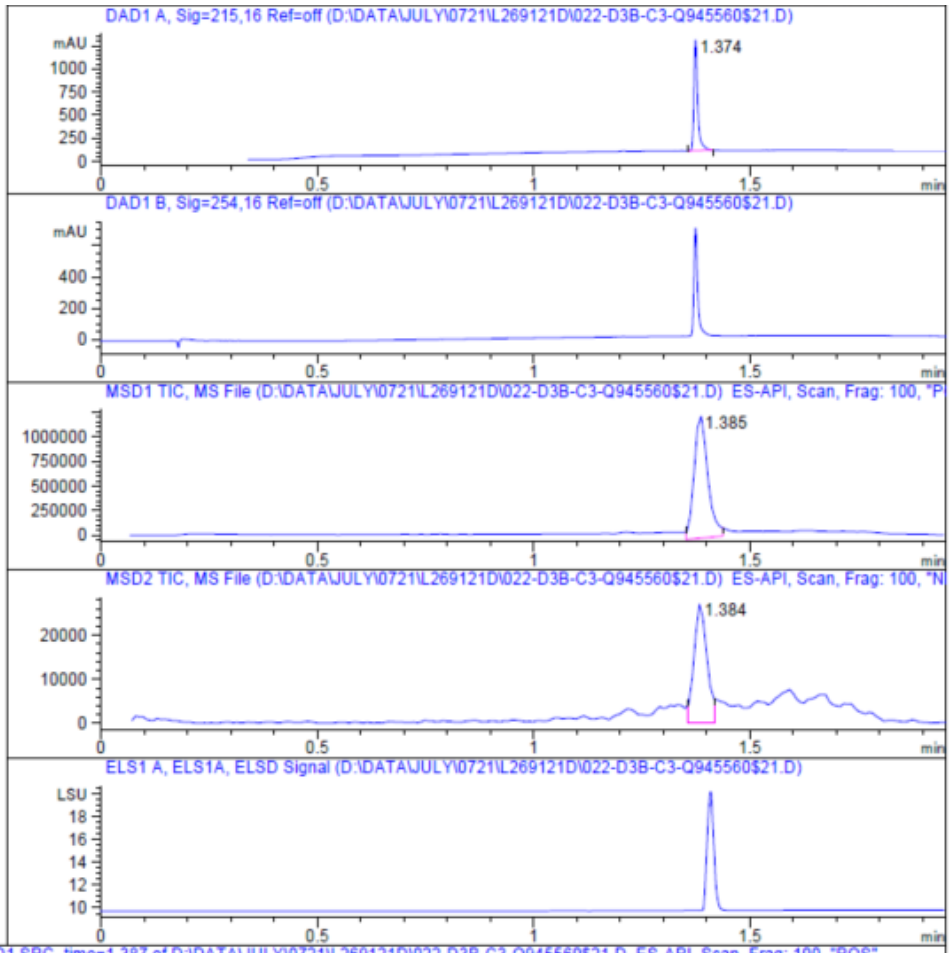


LC/MS spectrum of 1{26,25,12}

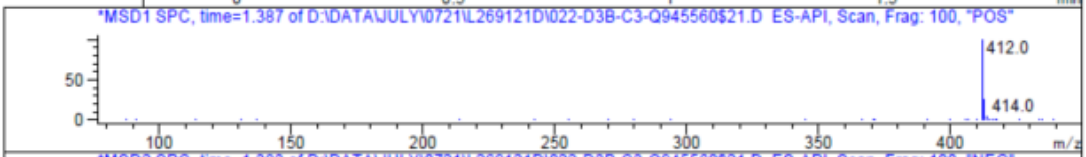


Mol Wt 411.46
Exact Mass 411.19

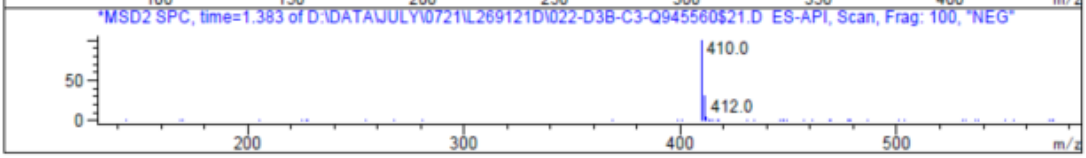
#	Time	Area%
1	1.374	100.00



RT 1.385

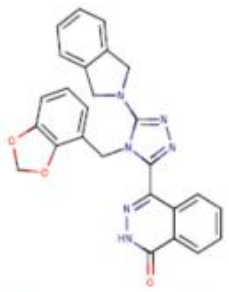


RT 1.384



LC/MS spectrum of 1{28,27,1}

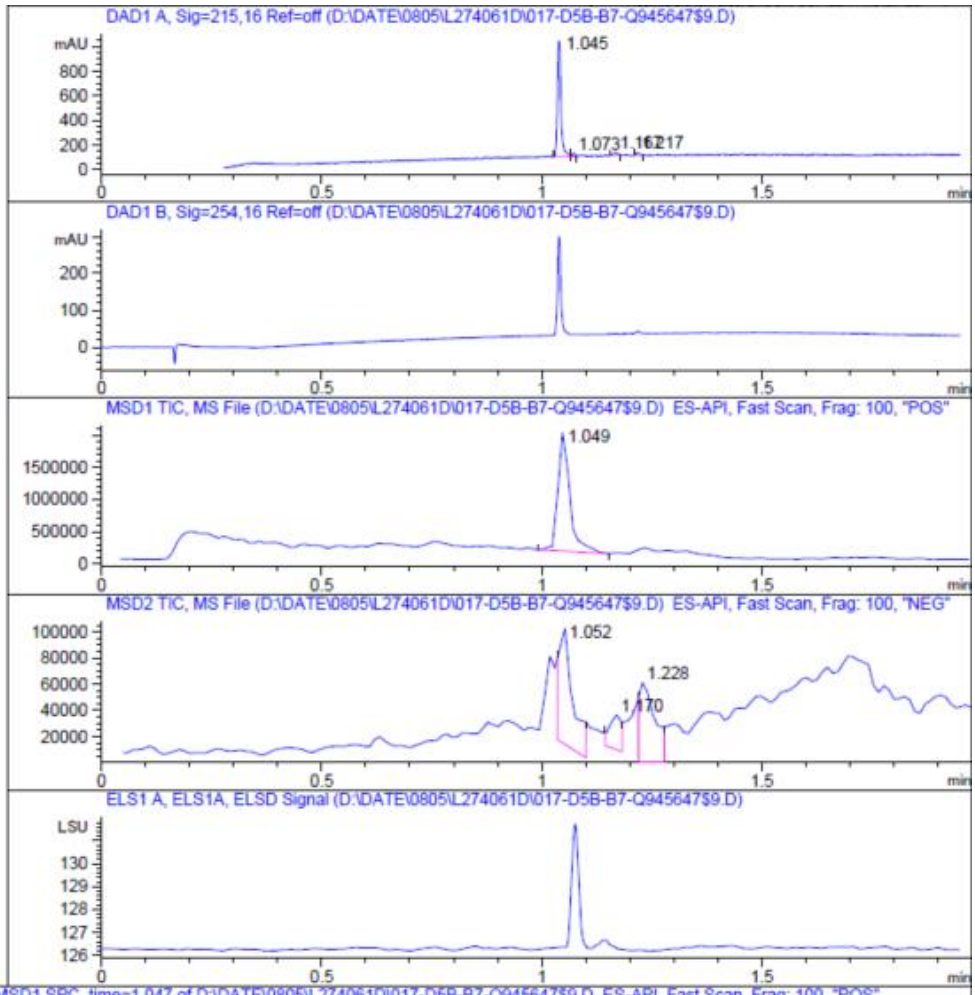
Ret_Time: 1.045 min



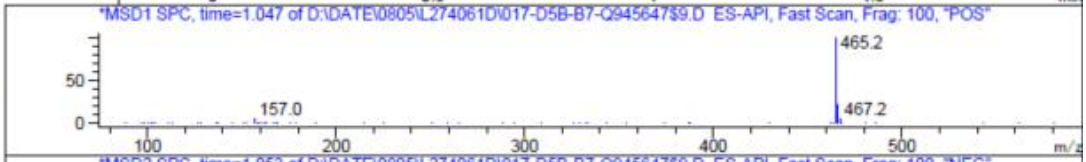
Mol Wt 464.48

Exact Mass 464.17

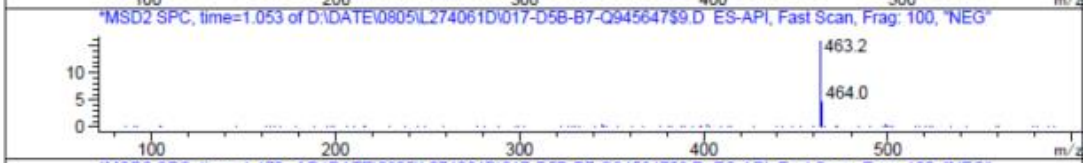
#	Time	Area%
1	1.045	92.94
2	1.073	2.59
3	1.167	2.46
4	1.217	2.01



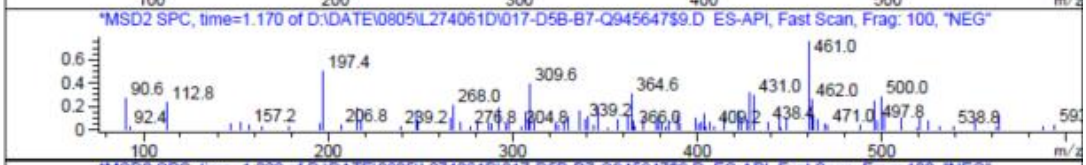
RT 1.049



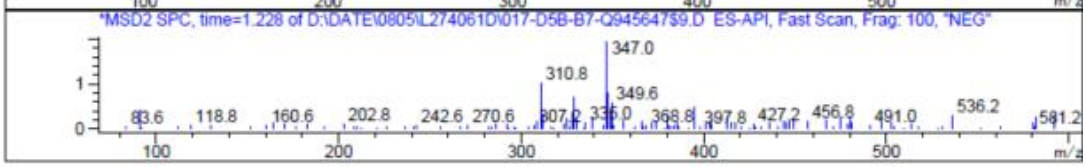
RT 1.052



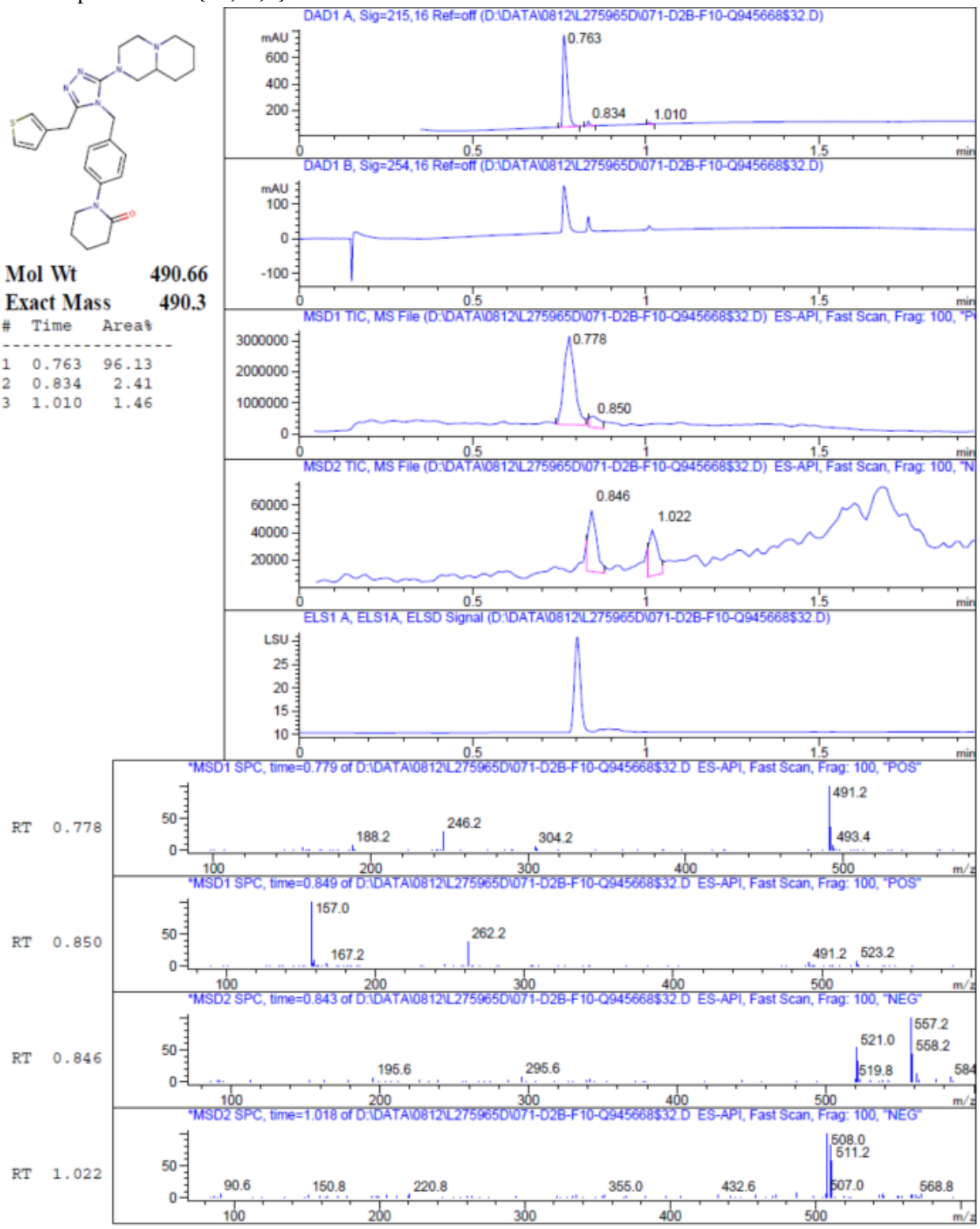
RT 1.170



RT 1.228

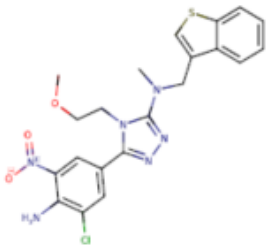


LC/MS spectrum of 1{29,28,4}



LC/MS spectrum of 1{30,29,14}

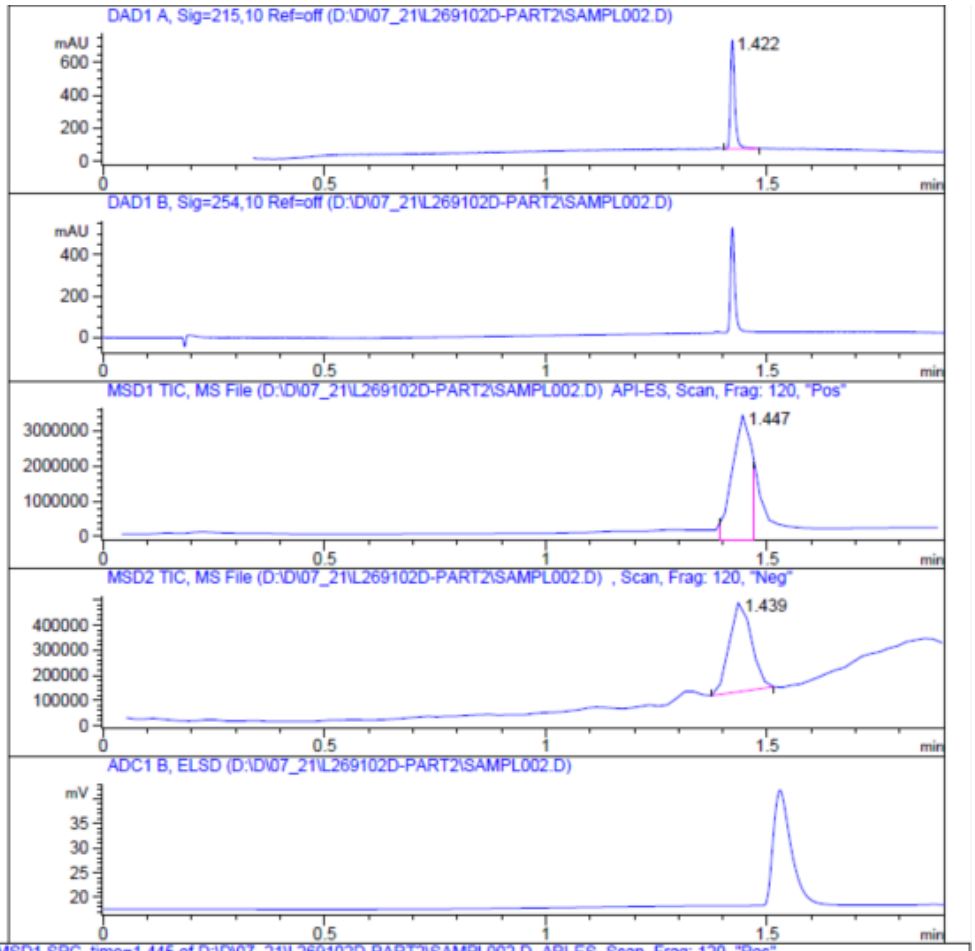
Ret_Time: 1.422 min



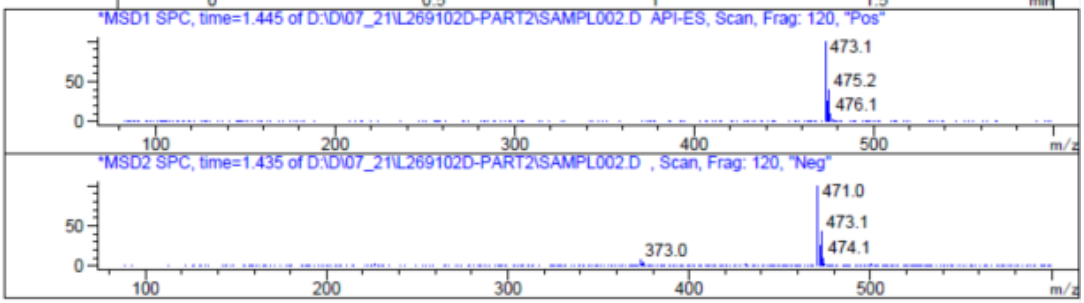
Mol Wt **472.95**

Exact Mass **472.12**

#	Time	Area%
1	1.422	100.00

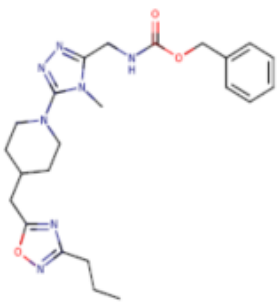


RT 1.447



RT 1.439

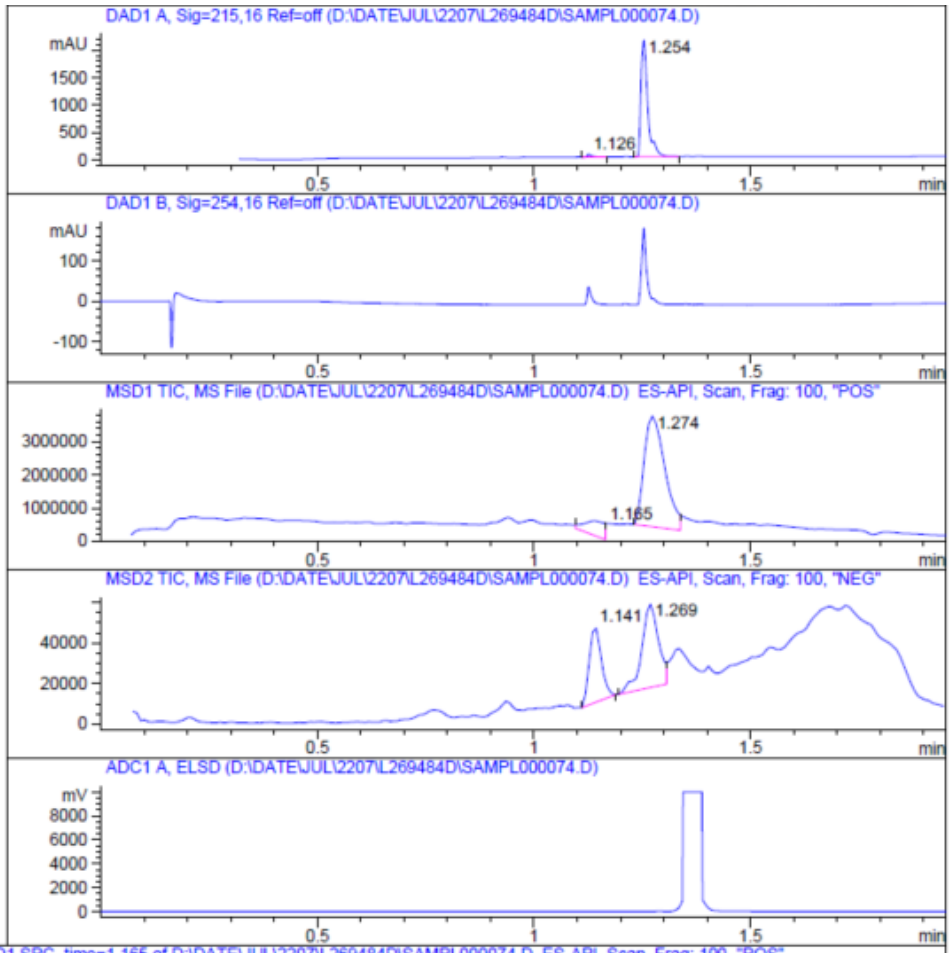
LC/MS spectrum of 1{31,30,9}



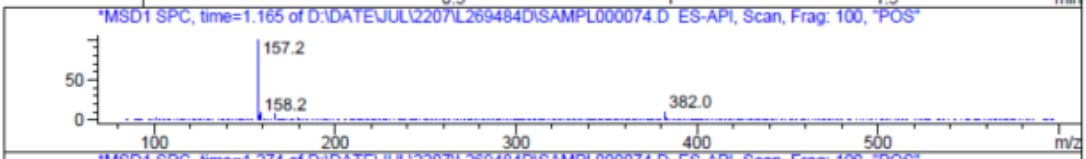
Mol Wt 453.54

Exact Mass 453.28

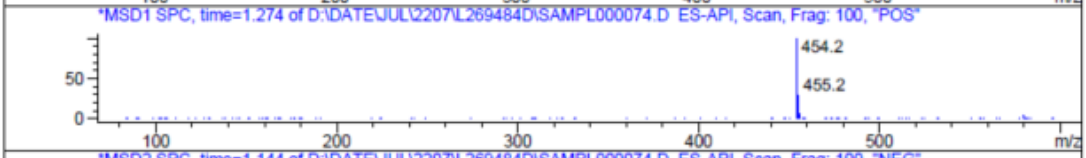
#	Time	Area%
1	1.126	1.59
2	1.254	98.41



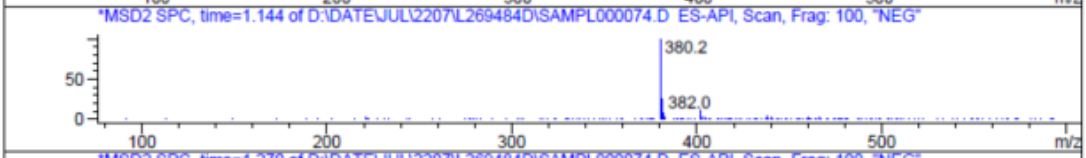
RT 1.165



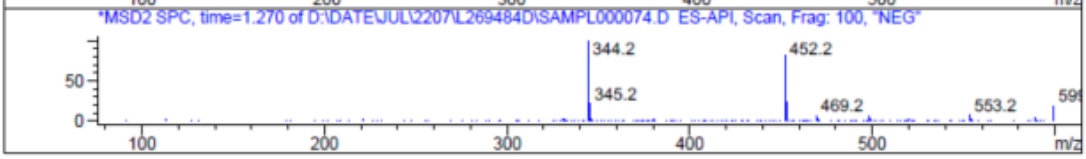
RT 1.274



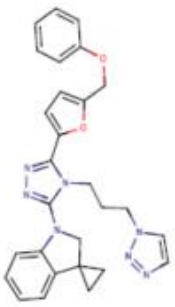
RT 1.141



RT 1.269



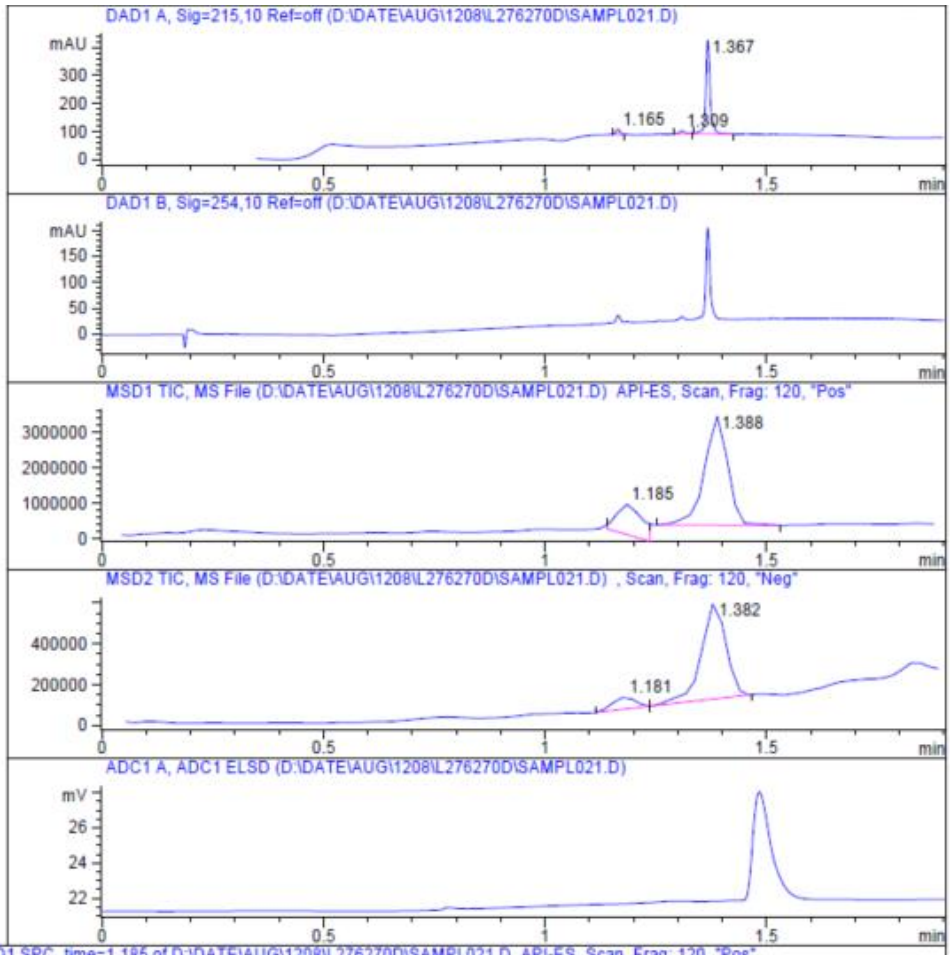
LC/MS spectrum of 1{32,31,15}



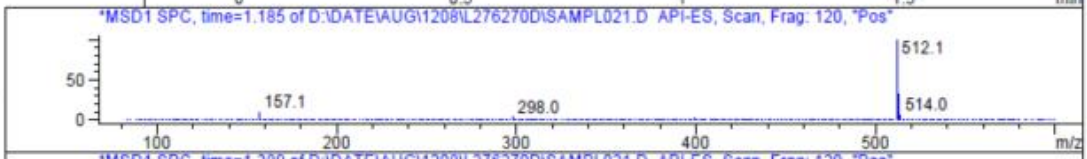
Mol Wt **493.56**

Exact Mass **493.25**

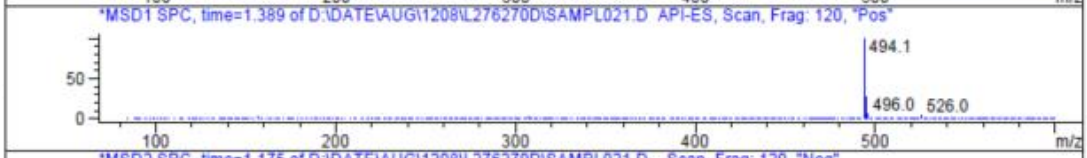
#	Time	Area%
1	1.165	4.68
2	1.309	3.58
3	1.367	91.74



RT 1.185

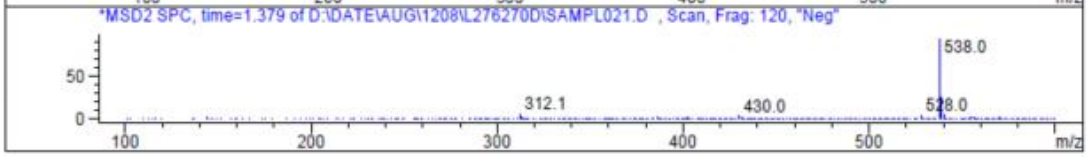


RT 1.388

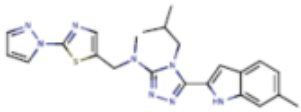


RT 1.181

RT 1.382



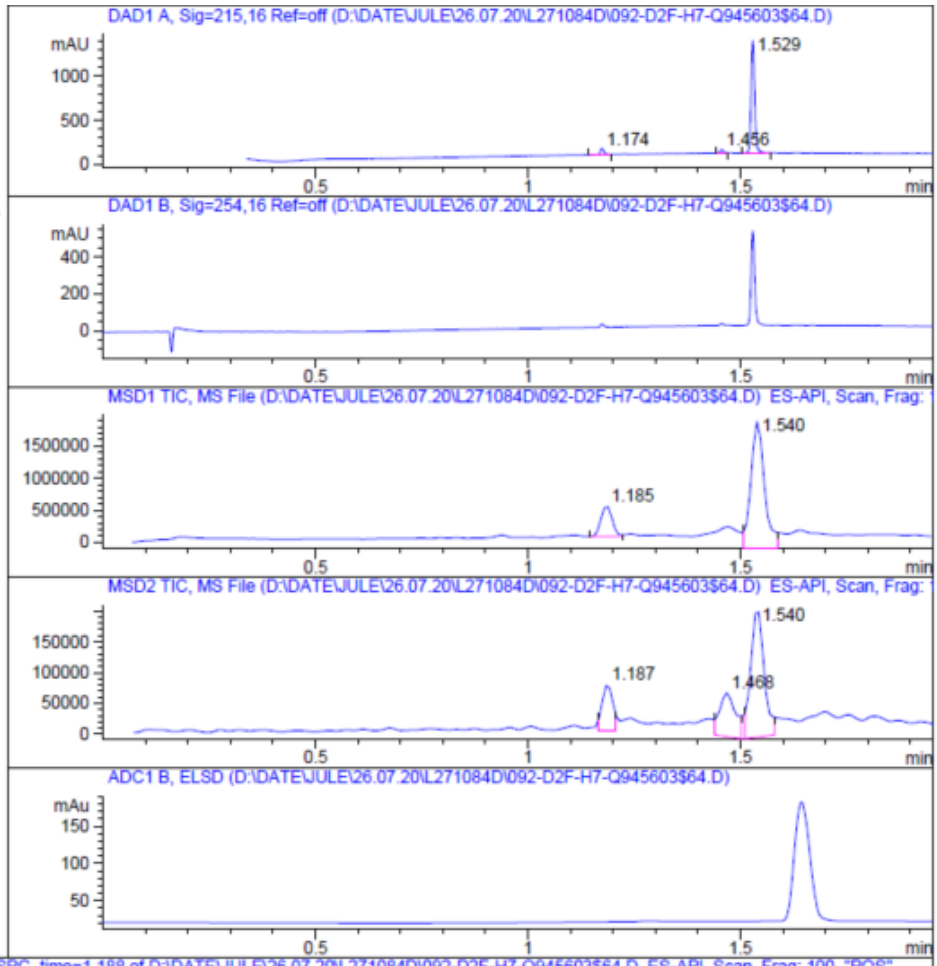
LC/MS spectrum of 1{35,34,16}

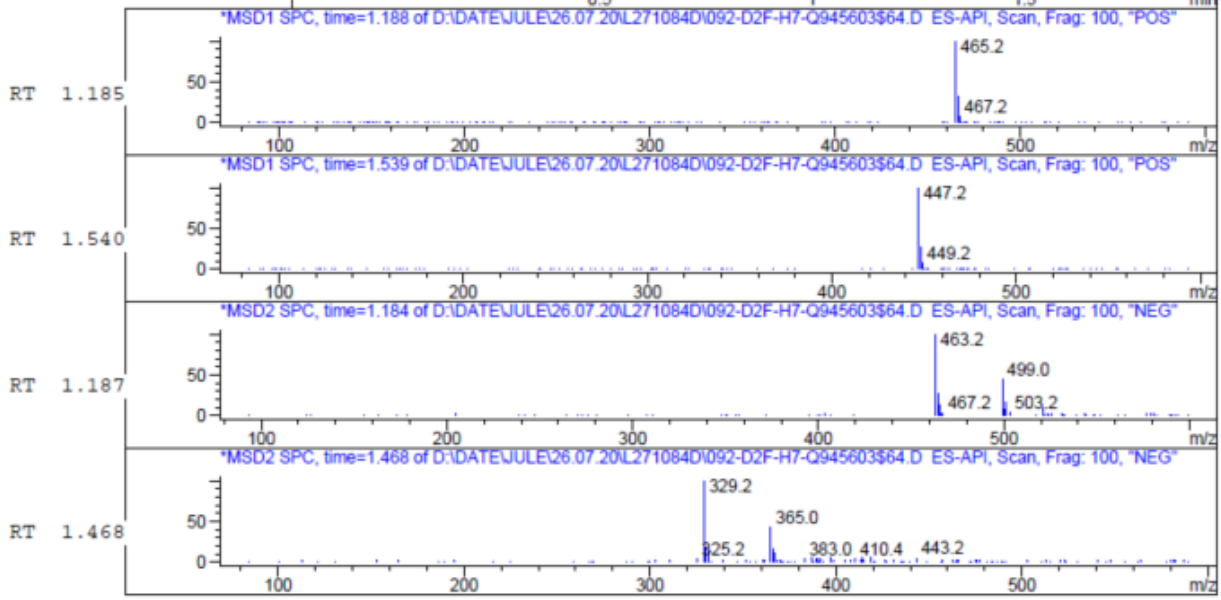


Mol Wt **446.57**

Exact Mass **446.23**

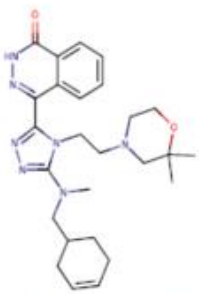
#	Time	Area%
1	1.174	5.30
2	1.456	2.58
3	1.529	92.11





LC/MS spectrum of 1{36,35,1}

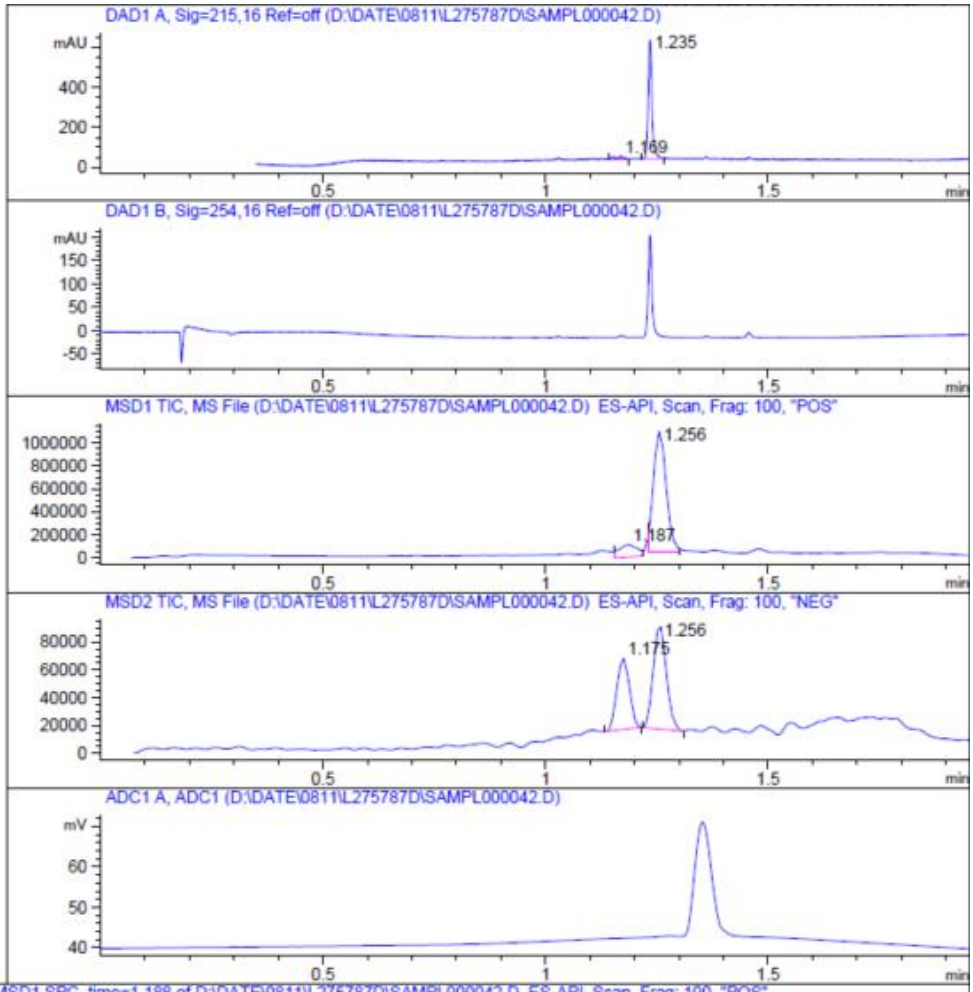
Ret_Time: 1.235 min



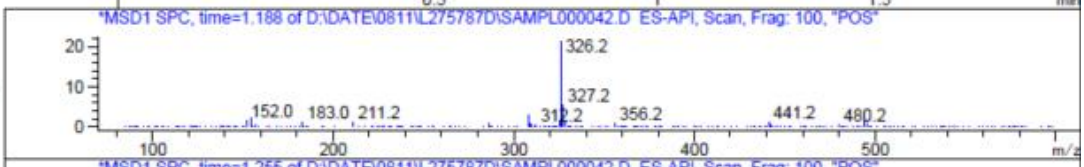
Mol Wt 477.6

Exact Mass 477.33

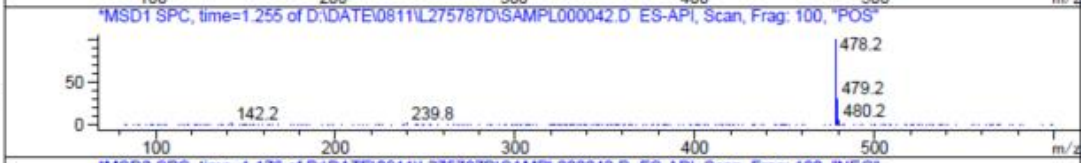
#	Time	Area%
1	1.169	5.38
2	1.235	94.62



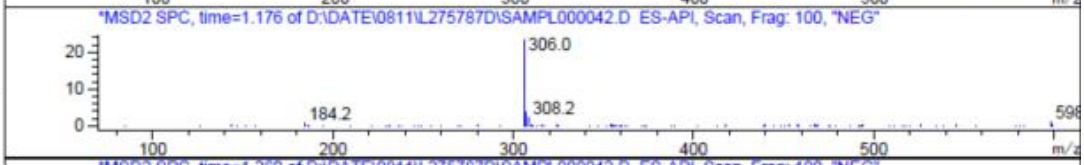
RT 1.187



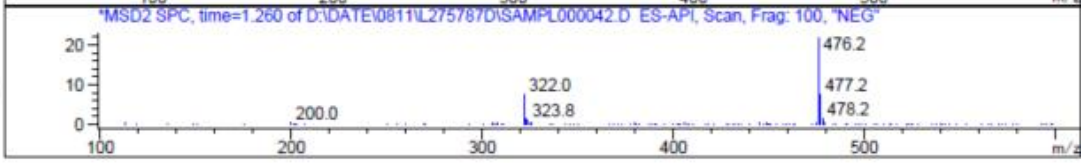
RT 1.256



RT 1.175

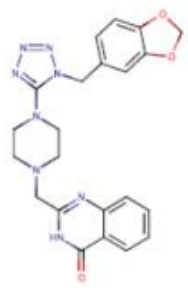


RT 1.256



LC/MS spectrum of 2{1,1}

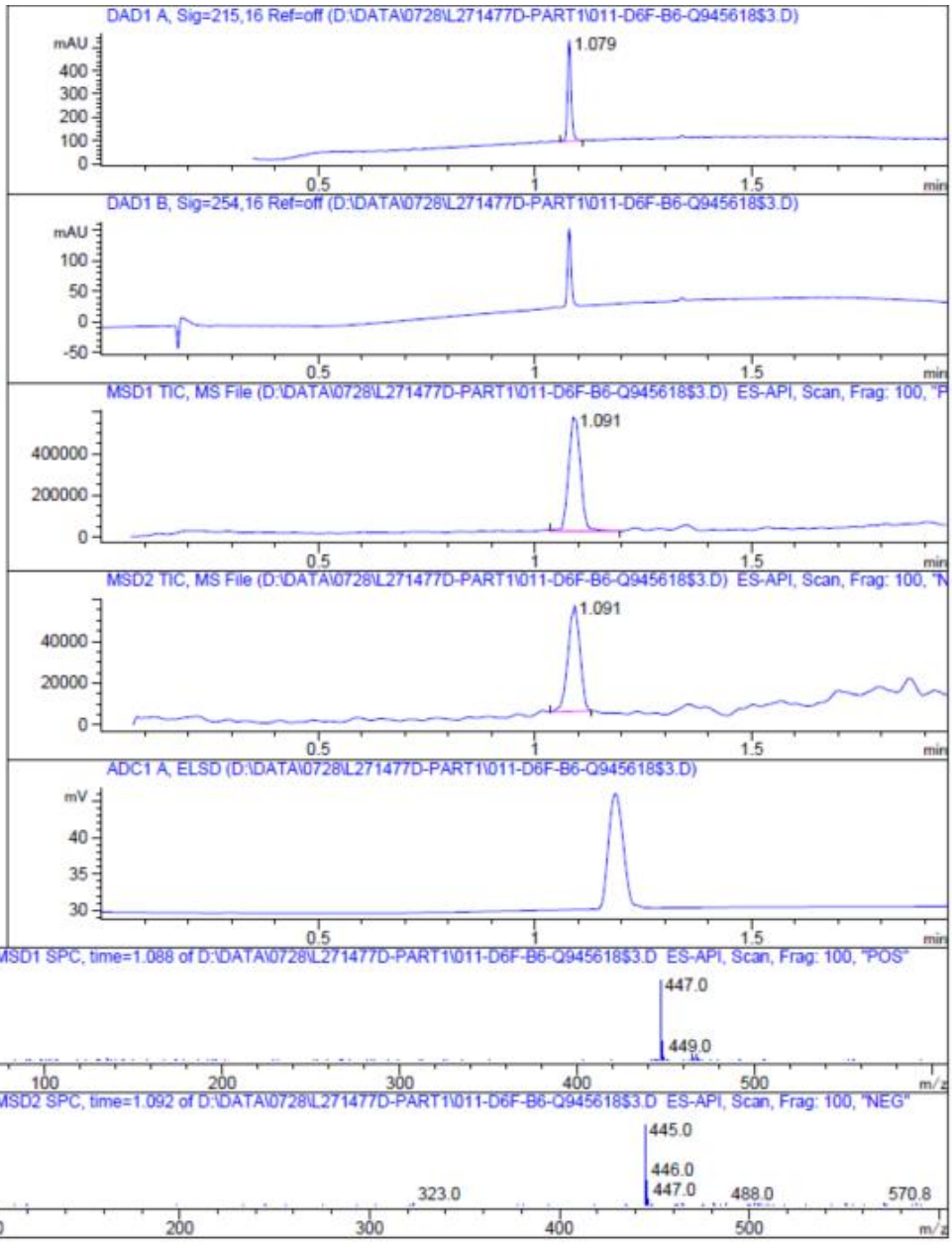
Ret_Time: 1.079 min



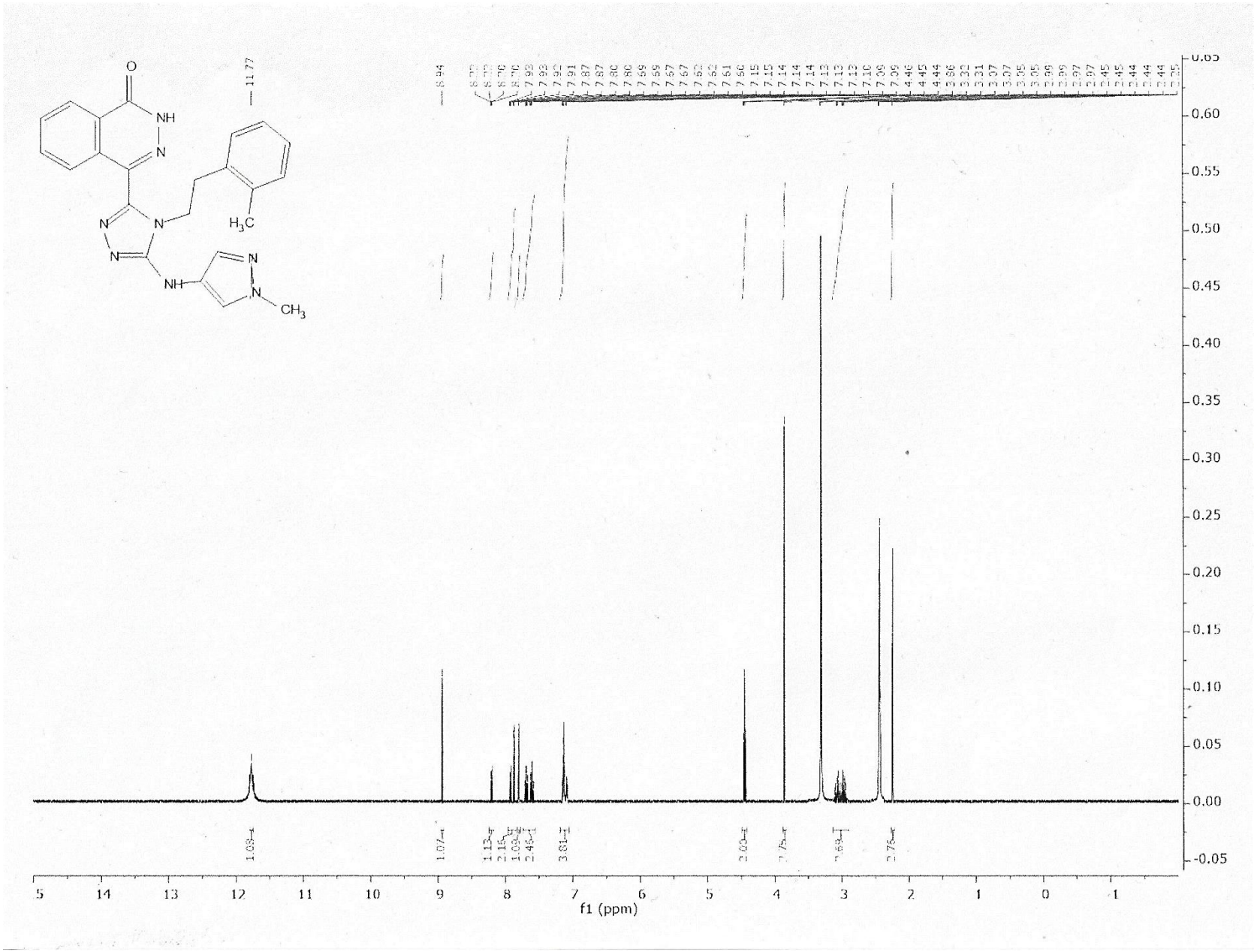
Mol Wt **446.46**

Exact Mass **446.19**

#	Time	Area%
1	1.079	100.00



^{1}H NMR spectrum of 1{9,9,1}



^{1}H NMR spectrum of 1{16,9,8}