

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102721\
 Data File : BF125973.D
 Acq On : 27 Oct 2021 20:21
 Operator : JU/CG
 Sample : M4348-04
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 358

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102521.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125973.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.122	3	6	12	rVB	2912832	3508543	80.62%	9.149%
2	5.075	505	508	515	rVB	50286	61618	1.42%	0.161%
3	5.469	570	575	578	rBV	4526703	4352106	100.00%	11.349%
4	6.481	741	747	750	rBV	4352166	4346706	99.88%	11.335%
5	6.857	805	811	814	rBV	1518343	1199891	27.57%	3.129%
6	7.416	901	906	909	rBV	3125482	2844673	65.36%	7.418%
7	8.010	1003	1007	1009	rBV	69049	67055	1.54%	0.175%
8	8.039	1009	1012	1018	rVB	754355	660925	15.19%	1.723%
9	8.139	1025	1029	1032	rBV	1824594	1503750	34.55%	3.921%
10	8.216	1039	1042	1051	rVB	482137	431412	9.91%	1.125%
11	9.216	1207	1212	1215	rBV	4669810	4014993	92.25%	10.470%
12	9.345	1229	1234	1243	rBV	335539	393995	9.05%	1.027%
13	9.622	1276	1281	1287	rBV3	35978	48283	1.11%	0.126%
14	9.892	1323	1327	1330	rVB	2093909	1647636	37.86%	4.296%
15	10.675	1456	1460	1464	rBV	2916371	2514956	57.79%	6.558%
16	10.816	1479	1484	1488	rVB2	49948	58785	1.35%	0.153%
17	10.904	1496	1499	1500	rBV2	46773	45156	1.04%	0.118%
18	10.928	1500	1503	1506	rVB	564213	460772	10.59%	1.202%
19	11.275	1559	1562	1566	rVB2	48391	64798	1.49%	0.169%
20	11.375	1575	1579	1581	rBV	1977017	1608360	36.96%	4.194%
21	11.398	1581	1583	1586	rVV	359859	276281	6.35%	0.720%
22	11.445	1586	1591	1595	rVB3	84373	94455	2.17%	0.246%
23	11.775	1644	1647	1654	rVB2	59406	49719	1.14%	0.130%
24	11.904	1666	1669	1673	rVB	94973	77462	1.78%	0.202%
25	11.986	1680	1683	1685	rBV	70031	67494	1.55%	0.176%
26	12.427	1755	1758	1762	rBV2	82222	88259	2.03%	0.230%
27	12.586	1781	1785	1788	rVB	419946	356971	8.20%	0.931%
28	12.810	1817	1823	1827	rBV	330951	362877	8.34%	0.946%
29	12.963	1845	1849	1852	rBV	3550223	3029407	69.61%	7.900%
30	13.863	1999	2002	2010	rVB2	271688	328051	7.54%	0.855%
31	14.010	2022	2027	2030	rBV2	1439488	1570852	36.09%	4.096%
32	14.033	2030	2031	2037	rVB	167714	113013	2.60%	0.295%
33	14.498	2108	2110	2115	rBV5	34055	50141	1.15%	0.131%
34	14.880	2171	2175	2179	rVB	269702	284034	6.53%	0.741%
35	15.045	2200	2203	2206	rBV	100582	140978	3.24%	0.368%
36	15.145	2218	2220	2224	rVB3	46015	44663	1.03%	0.116%

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ClientSampleId :
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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102521.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.345	2251	2254	2260	rVB	79501	112056	2.57%	0.292%
38	15.410	2262	2265	2269	rVB	87428	97497	2.24%	0.254%
39	15.474	2271	2276	2283	rBV	981763	1235721	28.39%	3.222%
40	15.962	2356	2359	2364	rVB4	35366	55841	1.28%	0.146%
41	16.021	2367	2369	2378	rVB9	44817	78539	1.80%	0.205%

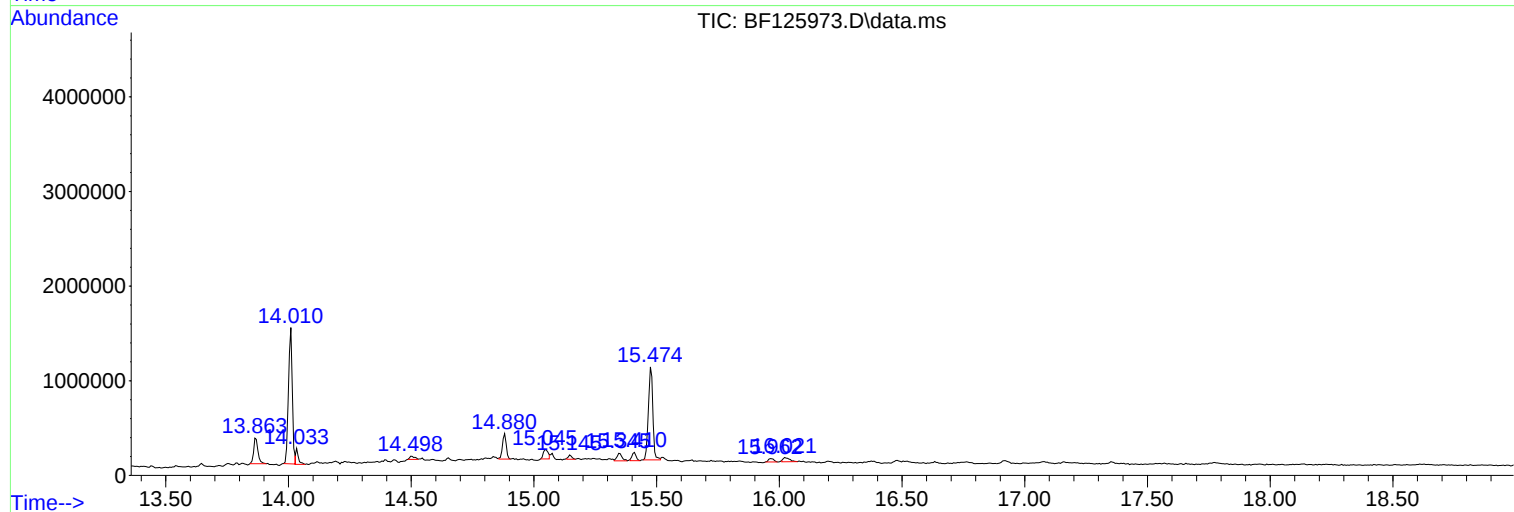
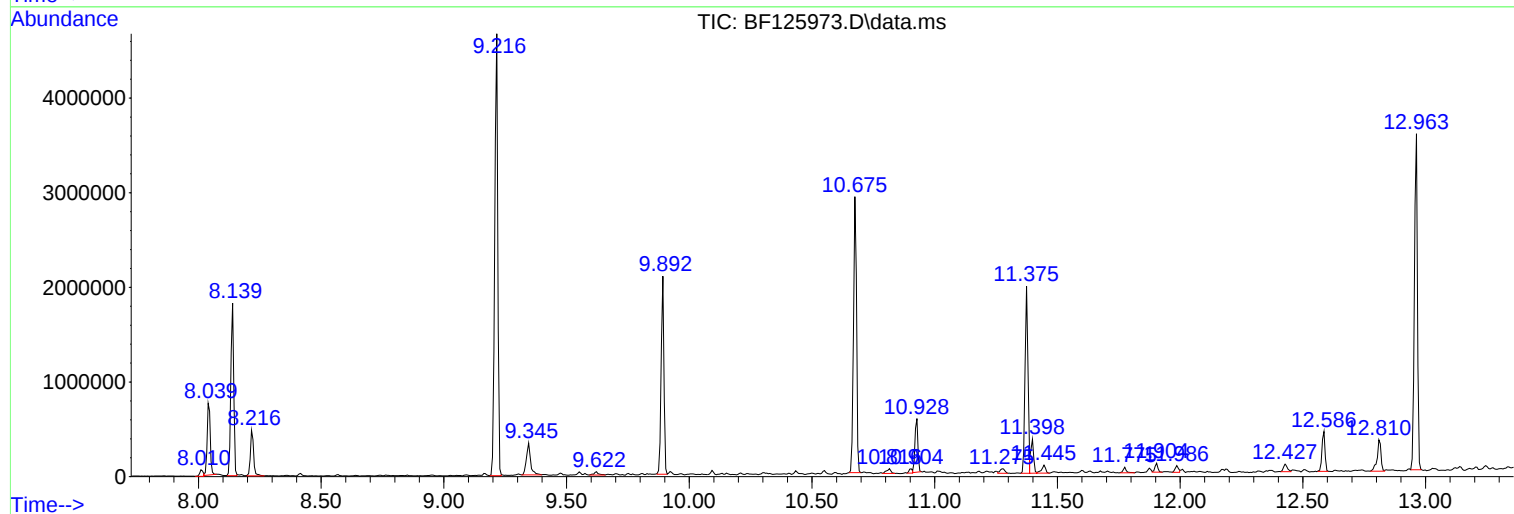
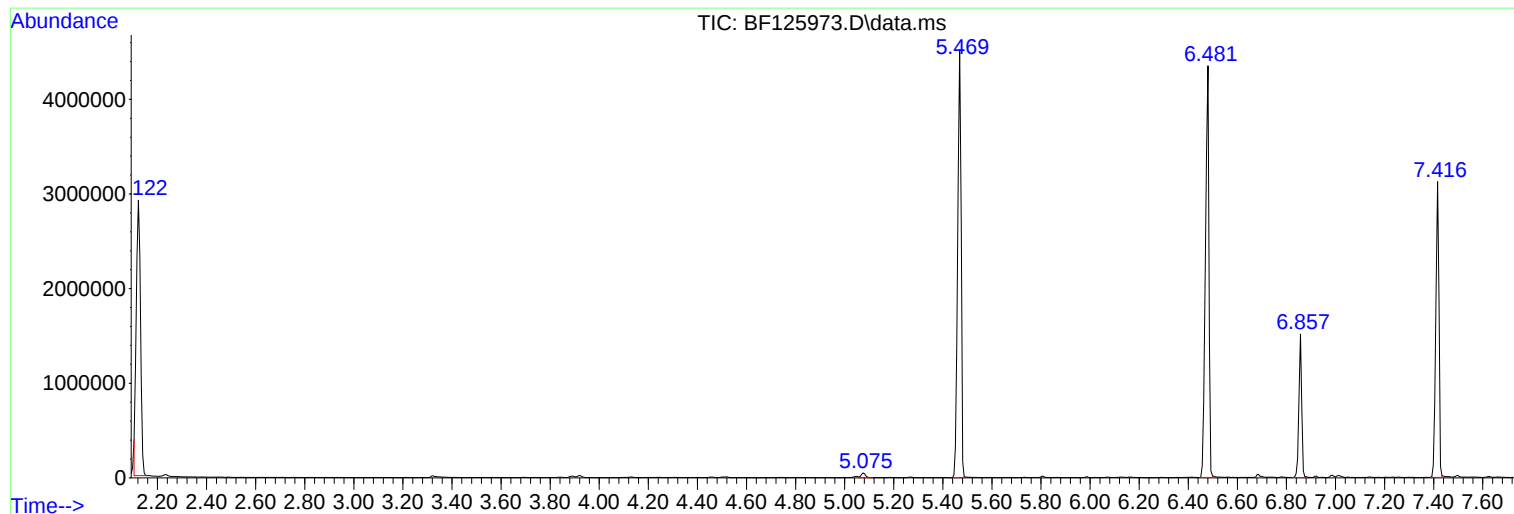
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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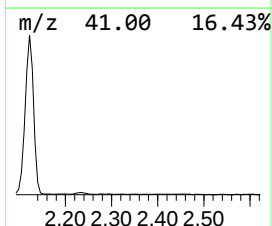
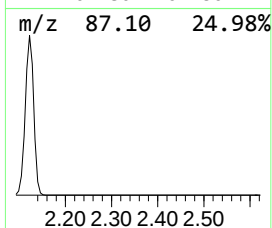
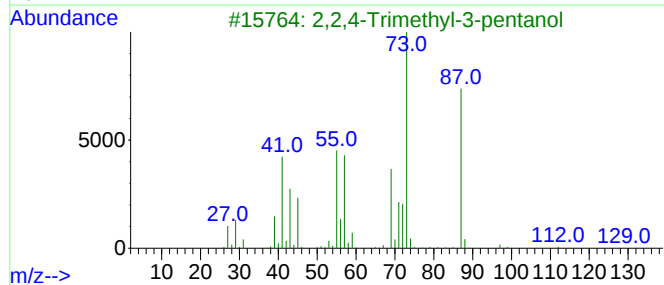
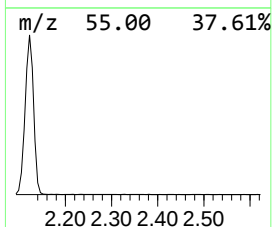
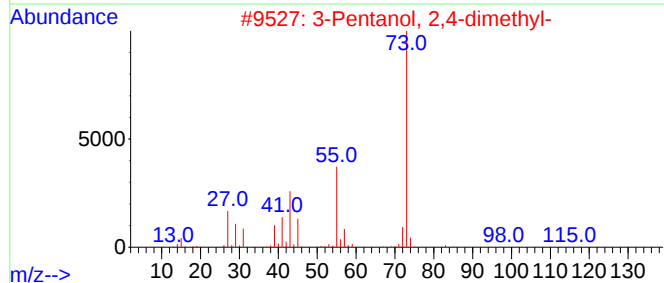
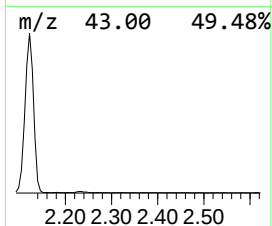
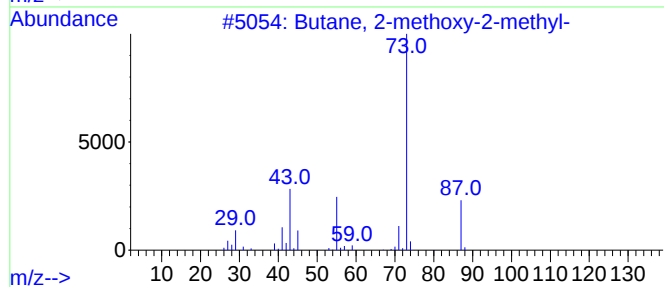
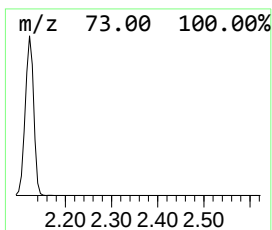
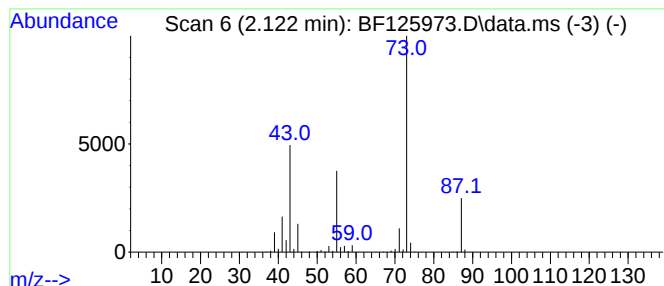
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.122	58.48 ng	3508540	1,4-Dichlorobenzene-d4	6.857

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	43
3			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
5			3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	17



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Sample : M4348-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
358

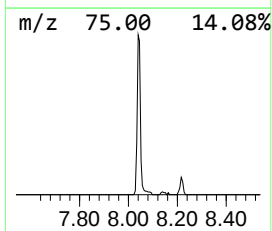
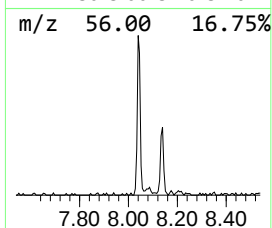
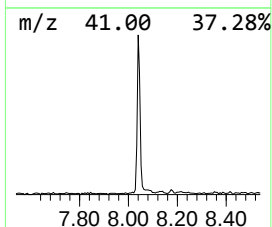
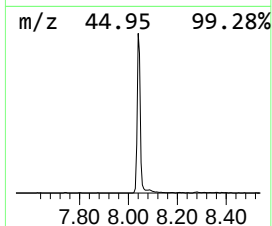
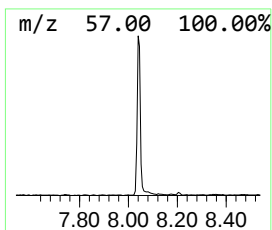
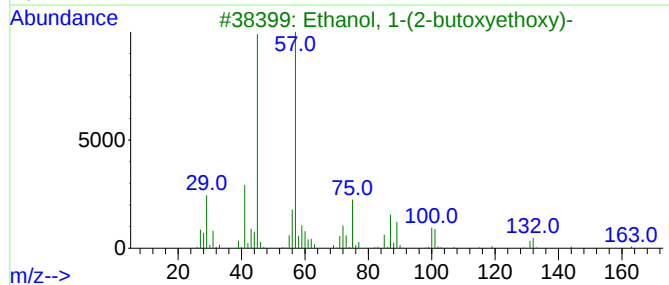
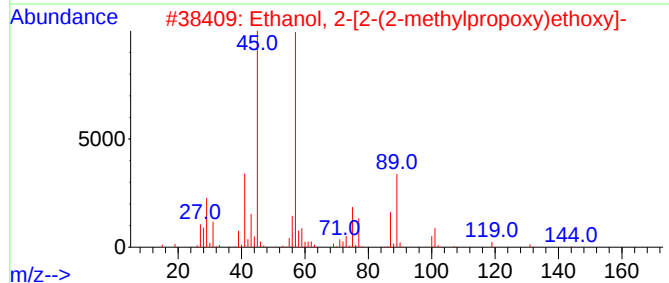
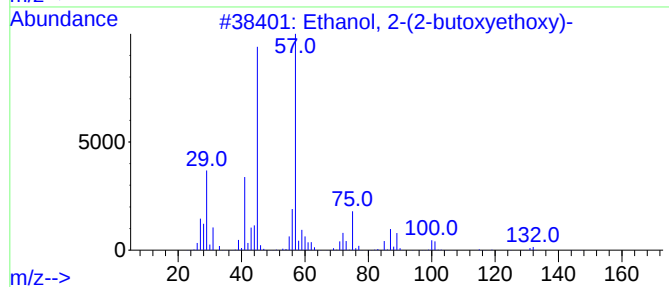
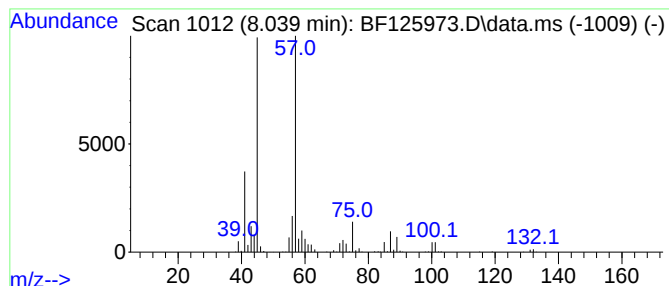
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.039	8.79 ng	660925	Naphthalene-d8	8.139

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
3			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	50
4			Tetraethylene glycol	194	C8H18O5	000112-60-7	50
5			Butyl lactate	146	C7H14O3	000138-22-7	47



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Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
358

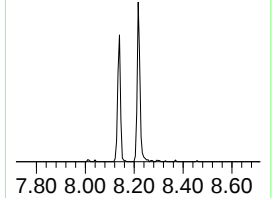
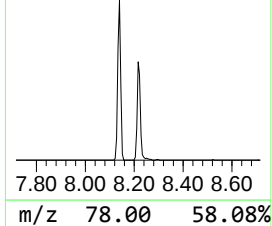
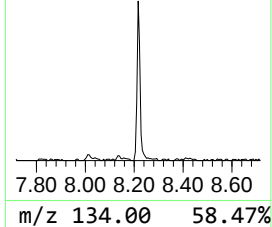
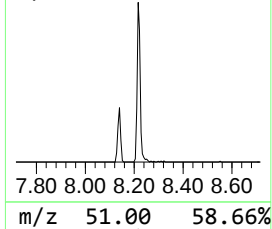
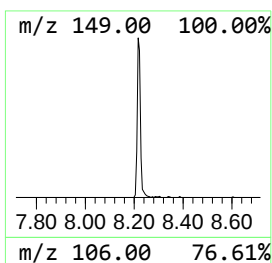
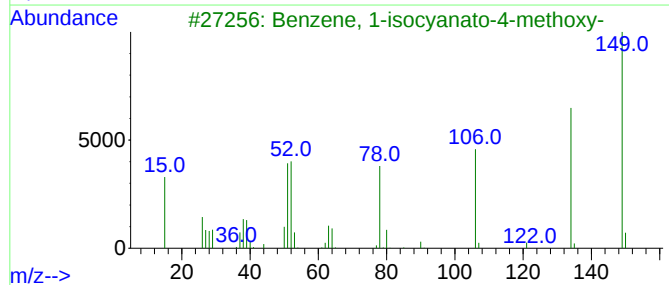
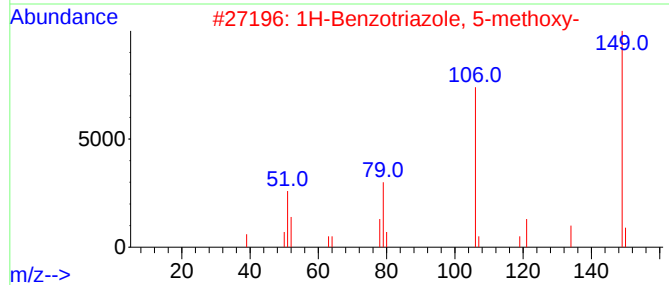
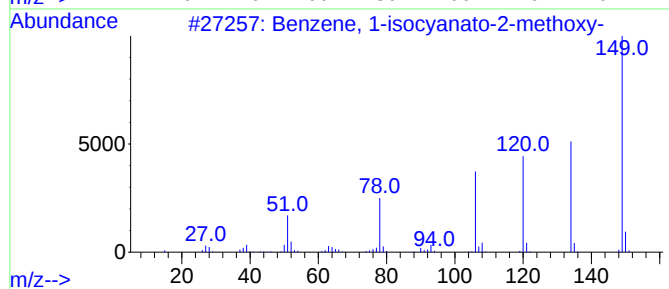
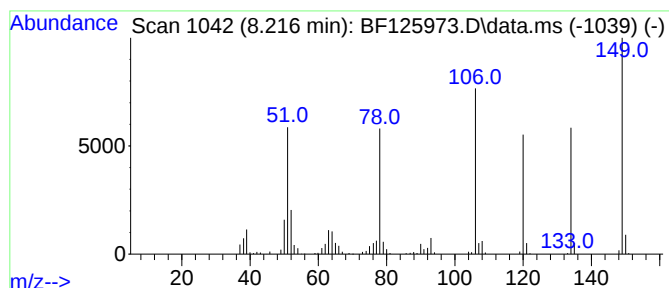
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzene, 1-isocyanato-2-met... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.216	5.74 ng	431412	Naphthalene-d8	8.139

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzene, 1-isocyanato-2-methoxy-	149	C8H7NO2	000700-87-8	95
2		1H-Benzotriazole, 5-methoxy-	149	C7H7N3O	027799-91-3	53
3		Benzene, 1-isocyanato-4-methoxy-	149	C8H7NO2	005416-93-3	49
4		Benzonitrile, 3-hydroxy-4-methoxy-	149	C8H7NO2	1000351-42-6	42
5		Benzonitrile, 4-hydroxy-3-methoxy-	149	C8H7NO2	004421-08-3	35



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ClientSampleId :
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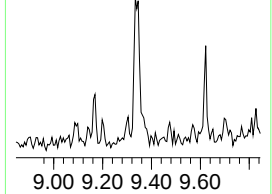
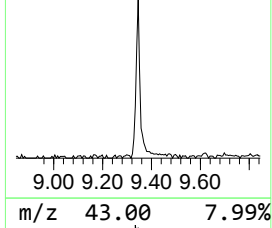
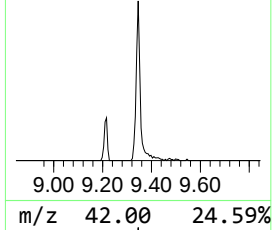
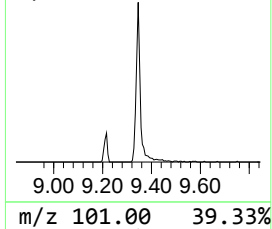
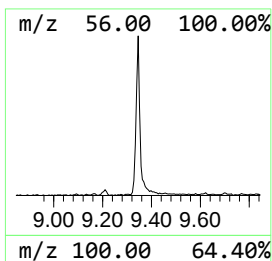
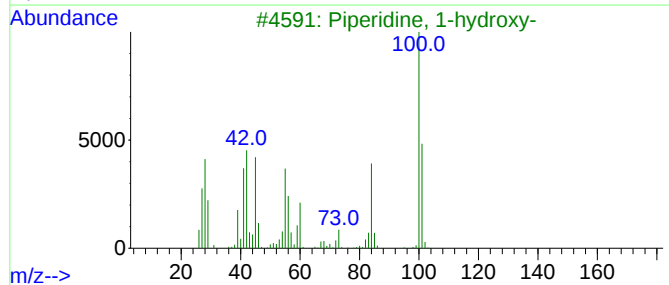
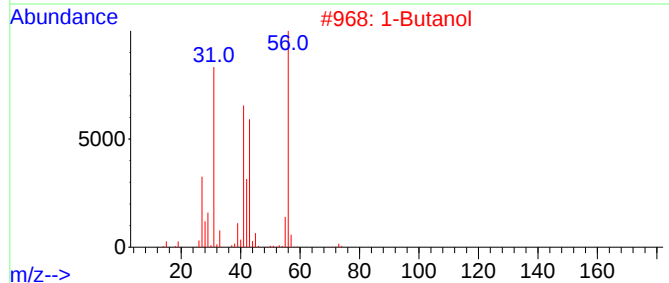
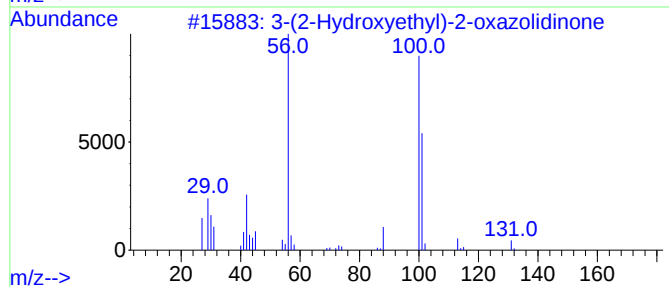
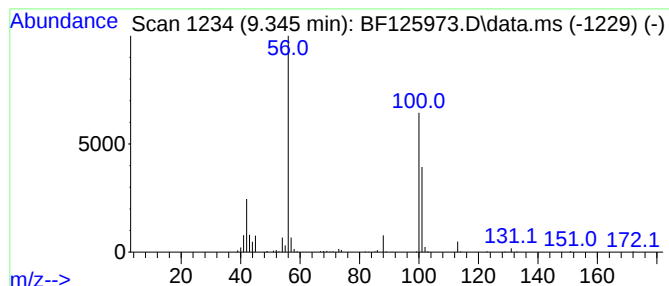
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 3-(2-Hydroxyethyl)-2-oxazol... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.345	4.78 ng	393995	Acenaphthene-d10	9.892

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-(2-Hydroxyethyl)-2-oxazolidinone	131	C5H9NO3	003356-88-5	83
2			1-Butanol	74	C4H10O	000071-36-3	38
3			Piperidine, 1-hydroxy-	101	C5H11NO	004801-58-5	25
4			Thiazolidine-2,4-dione, 5-dimeth...	172	C6H8N2O2S	175143-88-1	23
5			2,2,3,3,4,4,4-Heptafluoro-N-(2-m...	326	C10H13F7N2O2	1000278-15-3	17



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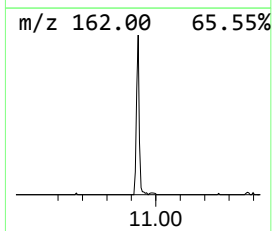
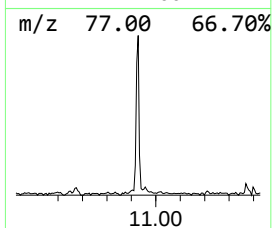
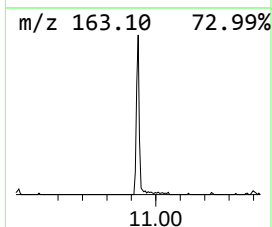
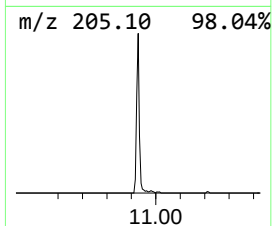
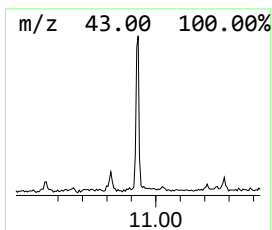
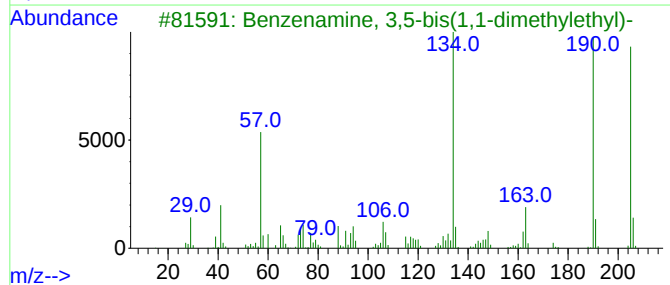
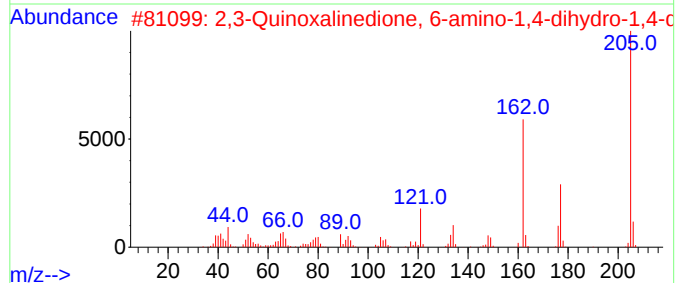
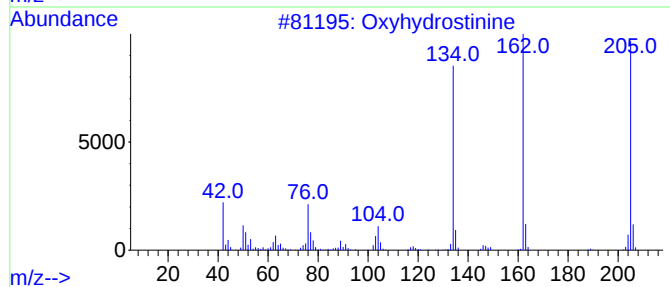
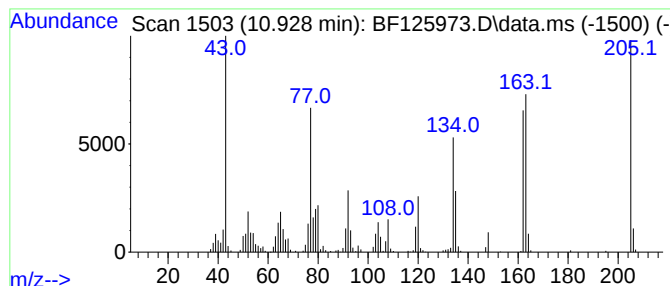
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Oxyhydrostinine Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.928	5.73 ng	460772	Phenanthrene-d10	11.374

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxyhydrostinine	205	C11H11NO3	000552-29-4	55
2			2,3-Quinoxalinedione, 6-amino-1,...	205	C10H11N3O2	1010338-06-6	35
3			Benzenamine, 3,5-bis(1,1-dimethy...	205	C14H23N	002380-36-1	27
4			Benzonitrile, 2,4-dimethoxy-	163	C9H9NO2	004107-65-7	22
5			(1E)-2-Propenal (4-nitrophenyl)h...	205	C10H11N3O2	1000507-14-3	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102721\
Data File : BF125973.D
Acq On : 27 Oct 2021 20:21
Operator : JU/CG
Sample : M4348-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

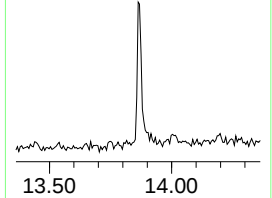
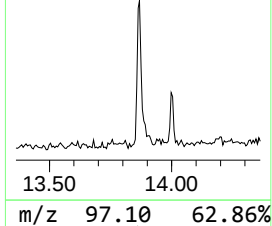
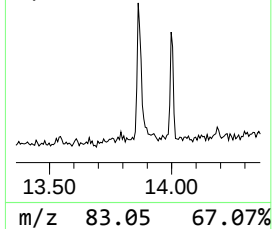
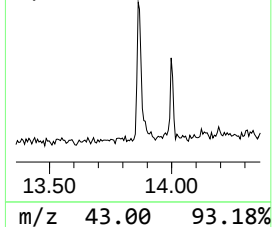
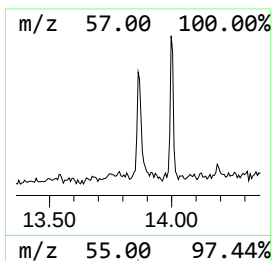
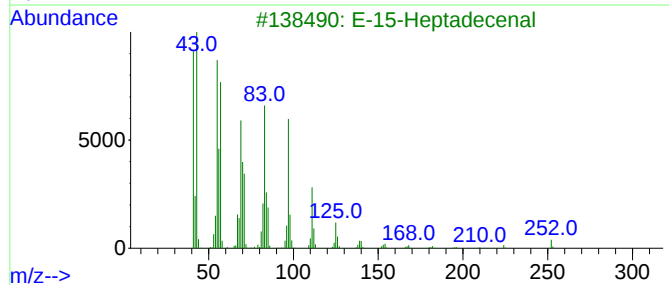
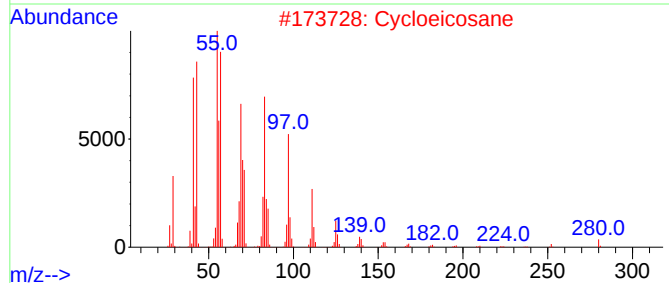
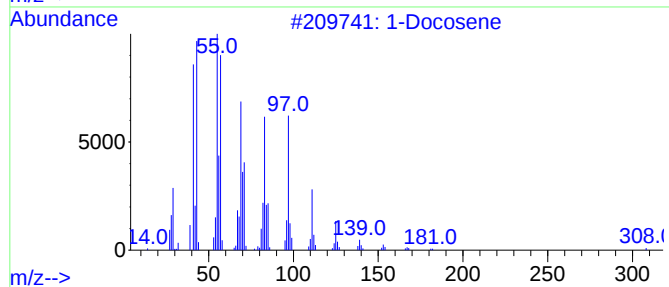
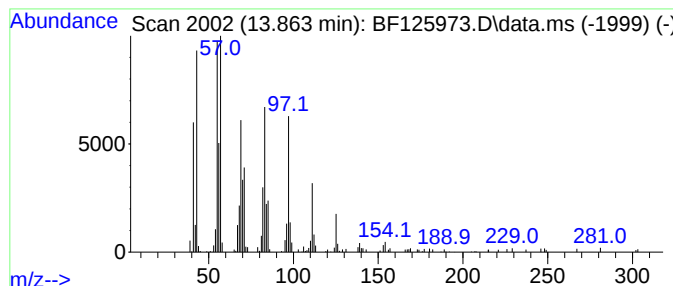
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 1-Docosene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.863	4.18 ng	328051	Chrysene-d12	14.010	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	94
2	Cycloeicosane	280	C20H40	000296-56-0	91
3	E-15-Heptadecenal	252	C17H32O	1000130-97-9	91
4	Cyclotridecane	182	C13H26	000295-02-3	90
5	1-Tetracosene	336	C24H48	010192-32-2	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102721\
Data File : BF125973.D
Acq On : 27 Oct 2021 20:21
Operator : JU/CG
Sample : M4348-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
358

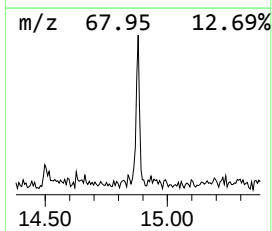
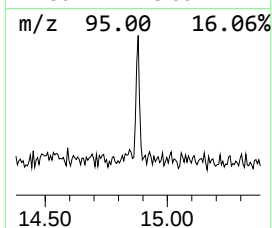
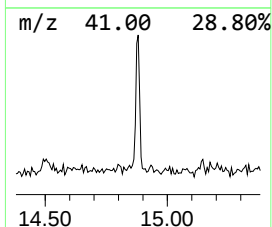
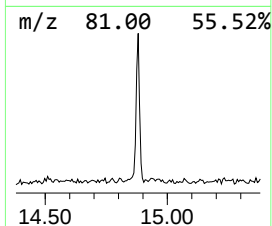
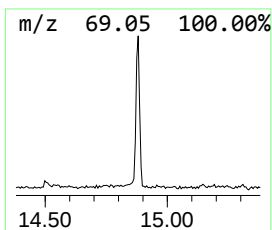
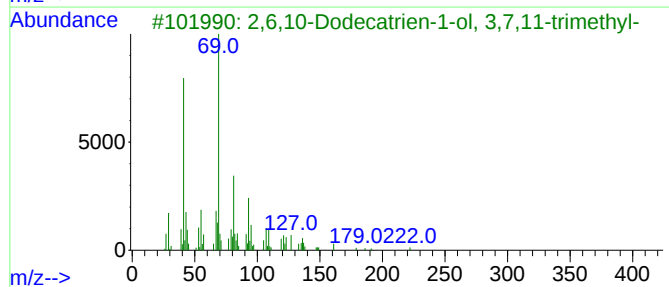
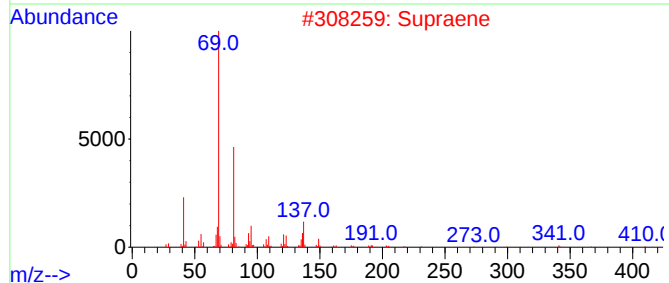
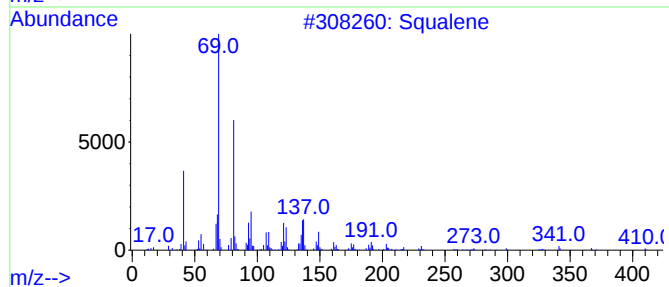
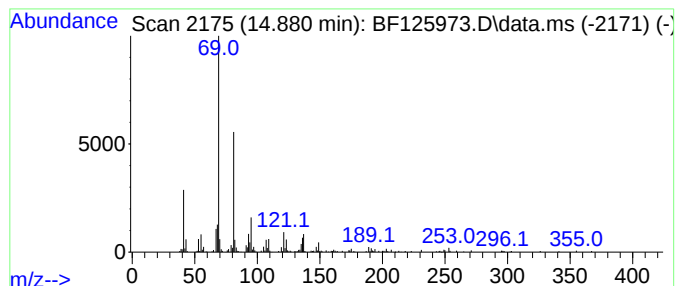
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Squalene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.880	4.60 ng	284034	Perylene-d12	15.474

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Squalene	410	C30H50	000111-02-4	90
2			Supraene	410	C30H50	007683-64-9	87
3			2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	59
4			3,7,11-Trimethyl-2,6,10-dodecatr...	217	C15H23N	029789-67-1	59
5			1,5,9-Decatriene, 2,3,5,8-tetram...	192	C14H24	230646-72-7	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102721\
Data File : BF125973.D
Acq On : 27 Oct 2021 20:21
Operator : JU/CG
Sample : M4348-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
358

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.122	58.5	ng	3508540	1	6.857	1199890	20.0
Ethanol, 2-(2-b...	8.039	8.8	ng	660925	2	8.139	1503750	20.0
Benzene, 1-isoc...	8.216	5.7	ng	431412	2	8.139	1503750	20.0
3-(2-Hydroxyeth...	9.345	4.8	ng	393995	3	9.892	1647640	20.0
Oxyhydrostinine	10.928	5.7	ng	460772	4	11.374	1608360	20.0
1-Docosene	13.863	4.2	ng	328051	5	14.010	1570850	20.0
Squalene	14.880	4.6	ng	284034	6	15.474	1235720	20.0