

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081518\
 Data File : BF108162.D
 Acq On : 15 Aug 2018 13:37
 Operator : JU/SJ
 Sample : J4447-36
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SP-1-10

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 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-BF080818.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.366	3	5	18	rVB	439043	585008	13.31%	1.440%
2	5.266	493	498	507	rVB	730834	904680	20.58%	2.226%
3	5.648	558	563	566	rBV	4040400	4123830	93.83%	10.148%
4	6.642	726	732	735	rBV	4313660	4395132	100.00%	10.816%
5	6.789	752	757	760	rBV	4683354	4340927	98.77%	10.683%
6	7.019	792	796	799	rVB	1344271	1099121	25.01%	2.705%
7	7.178	818	823	826	rBV	3418454	3175945	72.26%	7.816%
8	7.578	886	891	894	rBV	2746922	2834709	64.50%	6.976%
9	8.301	1010	1014	1017	rBV	1684992	1352377	30.77%	3.328%
10	9.377	1192	1197	1200	rBV	4208801	4156438	94.57%	10.229%
11	9.766	1259	1263	1266	rBV	594323	494375	11.25%	1.217%
12	9.972	1295	1298	1301	rVB	58275	48994	1.11%	0.121%
13	10.066	1308	1314	1317	rBV	1649070	1445512	32.89%	3.557%
14	10.472	1380	1383	1387	rVB	73860	61693	1.40%	0.152%
15	10.695	1417	1421	1424	rBV	56639	57768	1.31%	0.142%
16	10.860	1444	1449	1452	rBV	2701593	2677910	60.93%	6.590%
17	10.960	1461	1466	1470	rBV	127500	165144	3.76%	0.406%
18	11.401	1538	1541	1543	rBV	56210	50640	1.15%	0.125%
19	11.430	1543	1546	1549	rVB2	60101	59279	1.35%	0.146%
20	11.560	1564	1568	1571	rBV	1480770	1248957	28.42%	3.074%
21	12.060	1650	1653	1656	rBV3	44339	46656	1.06%	0.115%
22	13.013	1810	1815	1821	rBV2	49019	101068	2.30%	0.249%
23	13.148	1834	1838	1841	rBV	3683138	3092129	70.35%	7.609%
24	13.701	1929	1932	1935	rVB2	71787	60605	1.38%	0.149%
25	14.030	1985	1988	1995	rBV	375023	380786	8.66%	0.937%
26	14.218	2016	2020	2023	rBV	1121711	1082137	24.62%	2.663%
27	14.348	2039	2042	2047	rVB2	121789	119033	2.71%	0.293%
28	14.659	2092	2095	2103	rVB3	144633	202436	4.61%	0.498%
29	14.836	2122	2125	2128	rVB3	58045	58328	1.33%	0.144%
30	14.989	2148	2151	2154	rVB	128477	123683	2.81%	0.304%
31	15.071	2162	2165	2169	rVB	118419	115799	2.63%	0.285%
32	15.354	2210	2213	2217	rVB	144728	160666	3.66%	0.395%
33	15.783	2281	2286	2295	rVB2	935521	1388286	31.59%	3.416%
34	16.253	2362	2366	2372	rVB2	135351	208600	4.75%	0.513%

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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 >
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35	18.965	2821	2827	2828	rBV5	139782	216736	4.93%	0.533%
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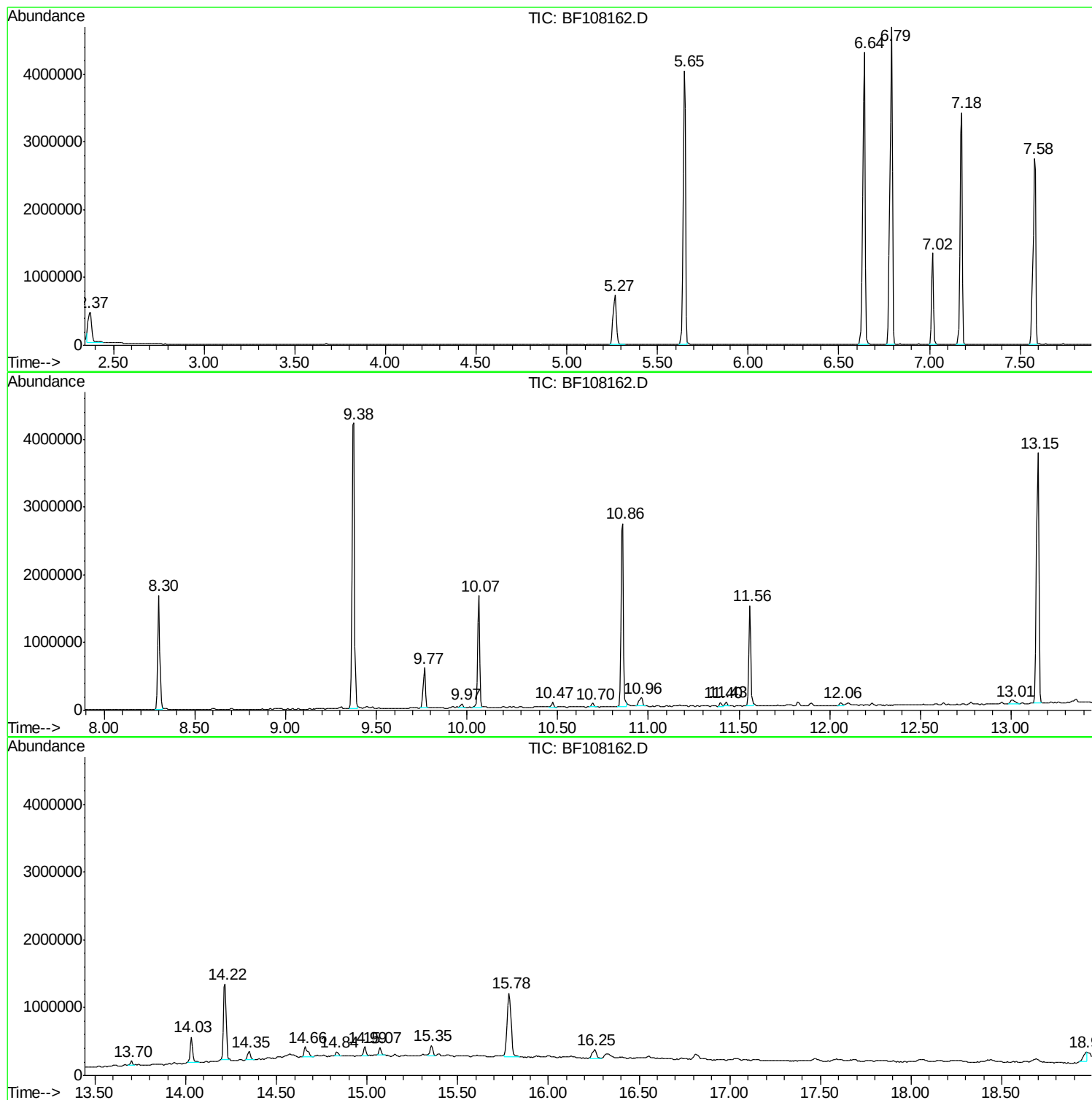
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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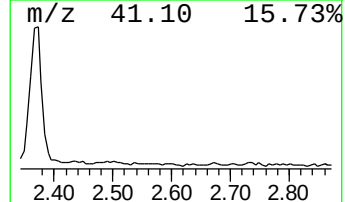
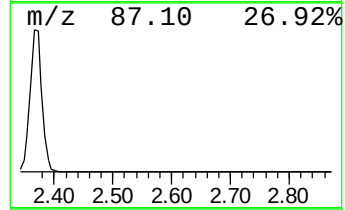
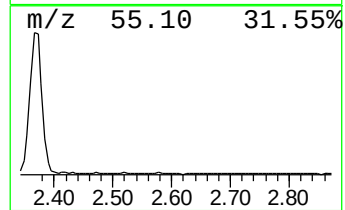
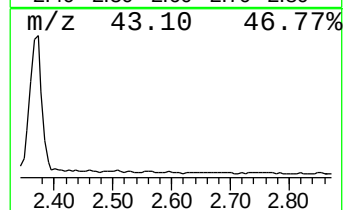
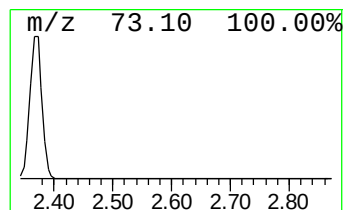
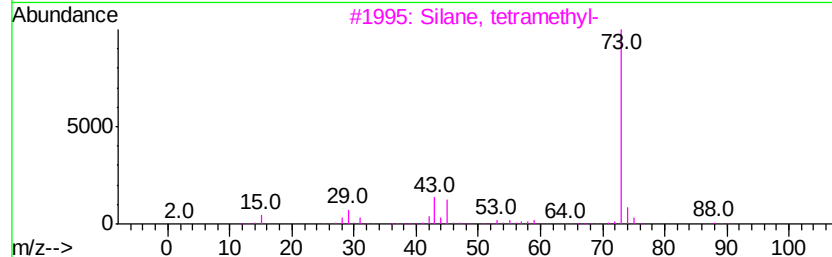
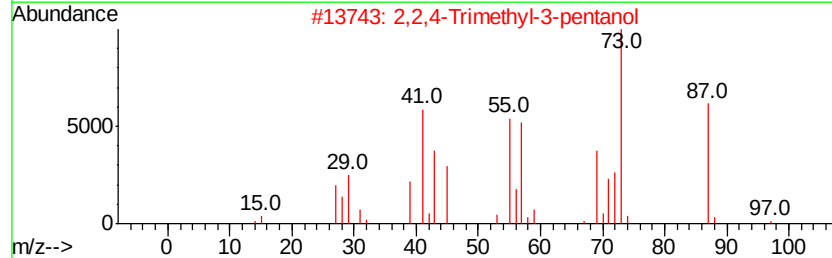
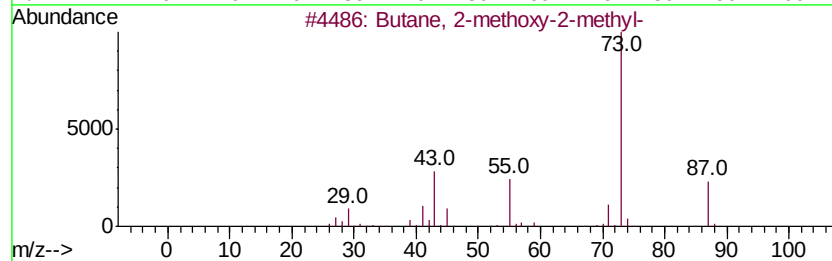
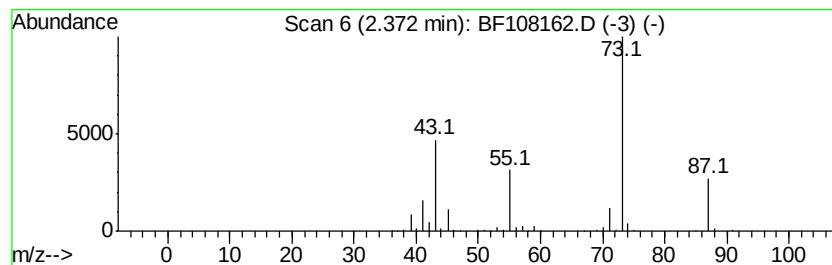
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.37	10.65 ng	585008	1,4-Dichlorobenzene-d4	7.02

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3		Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
4		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	32
5		2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	32



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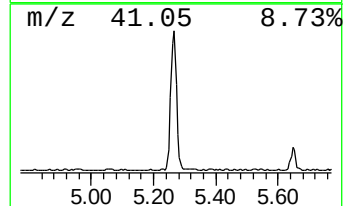
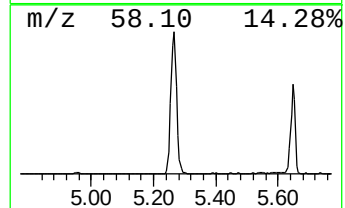
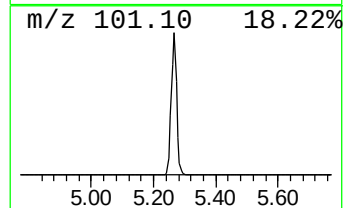
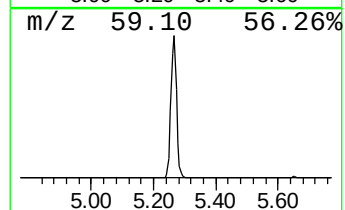
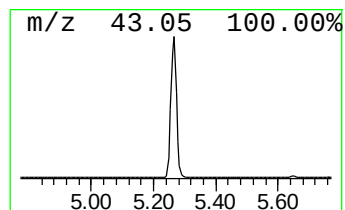
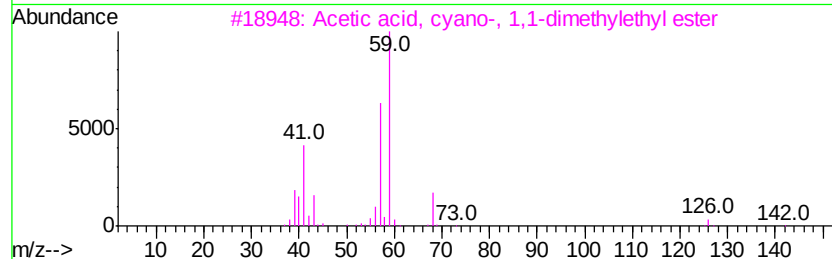
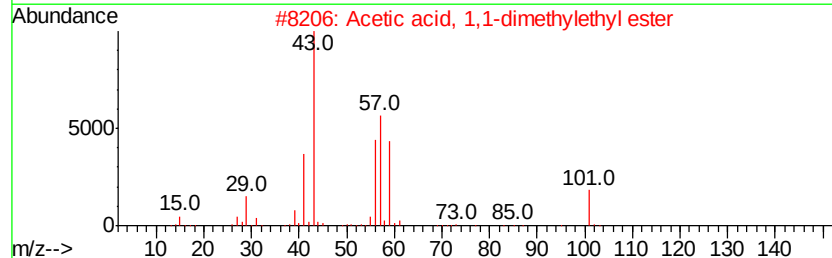
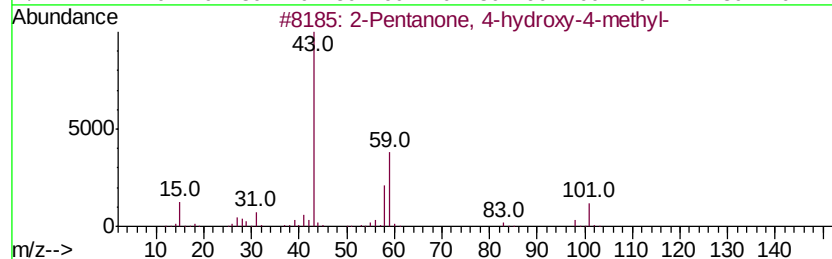
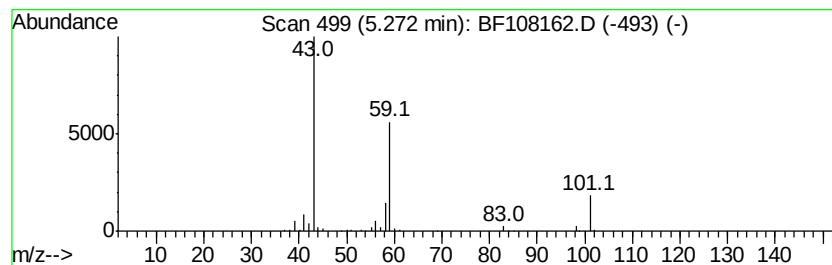
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.27	16.46 ng	904680	1,4-Dichlorobenzene-d4	7.02

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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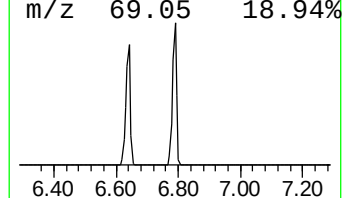
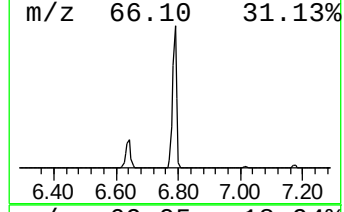
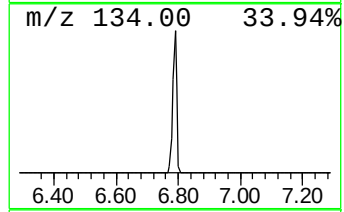
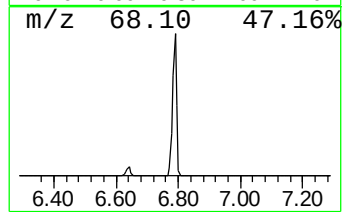
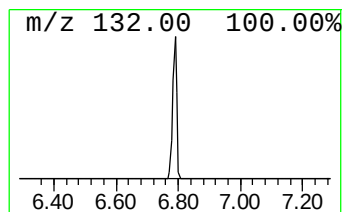
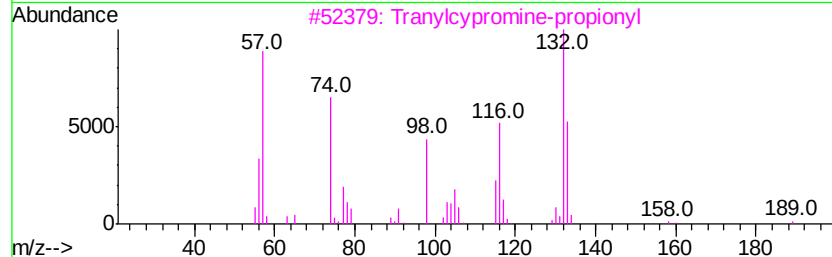
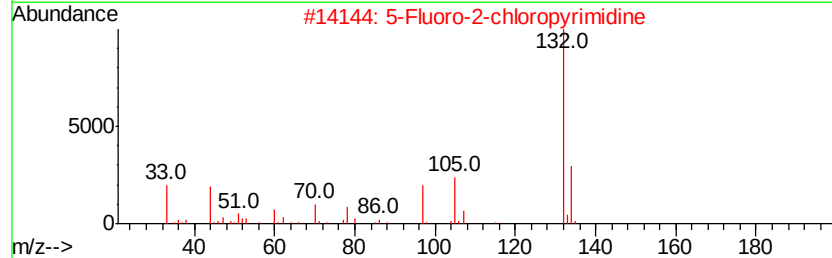
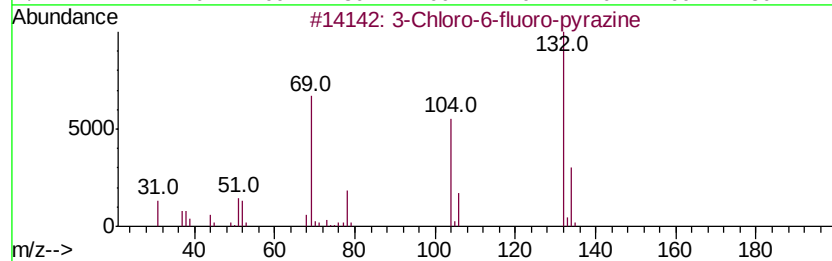
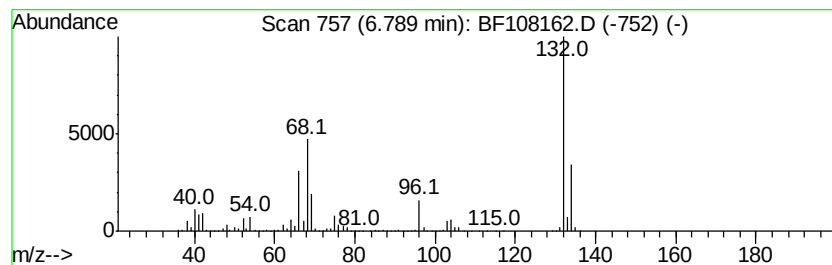
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.79 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.79	78.99 ng	4340930	1,4-Dichlorobenzene-d4	7.02

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
5		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9



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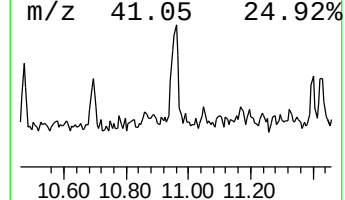
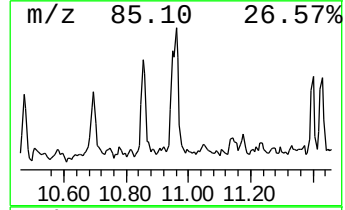
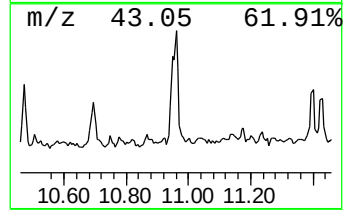
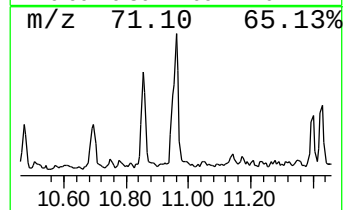
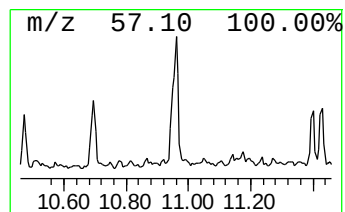
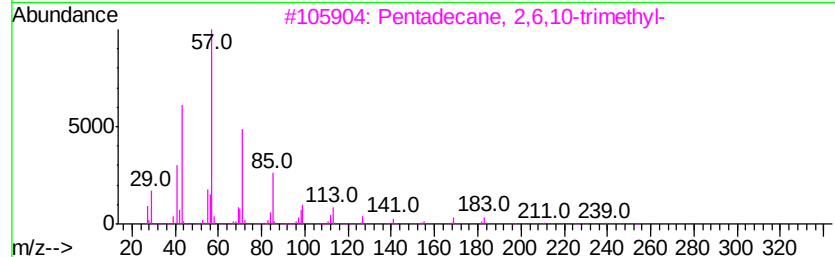
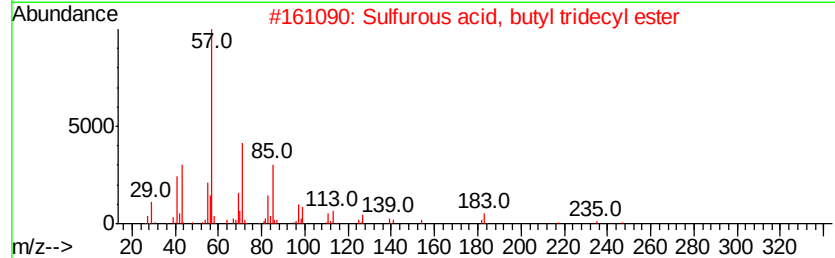
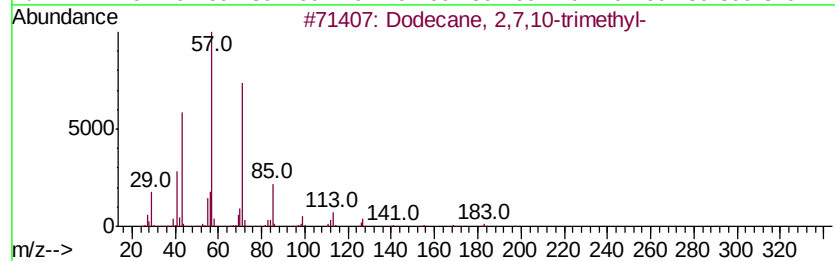
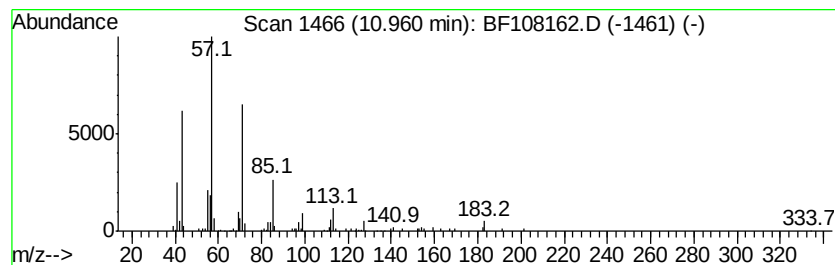
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Dodecane, 2,7,10-trimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.96	2.64 ng	165144	Phenanthrene-d10	11.56
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Dodecane, 2,7,10-trimethyl-	212 C15H32	074645-98-0	86
2	Sulfurous acid, butyl tridecyl e...	320 C17H36O3S	1000309-18-0	72
3	Pentadecane, 2,6,10-trimethyl-	254 C18H38	003892-00-0	72
4	Heptadecane, 2,6-dimethyl-	268 C19H40	054105-67-8	64
5	Sulfurous acid, 2-ethylhexyl und...	348 C19H40O3S	1000309-19-4	64



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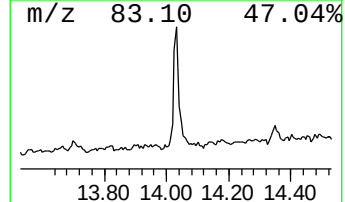
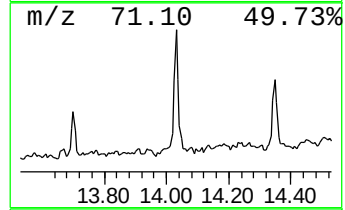
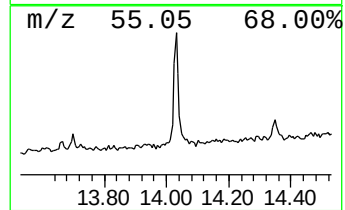
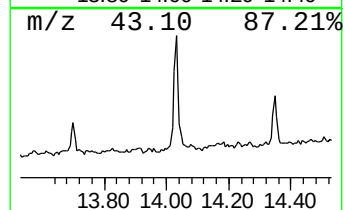
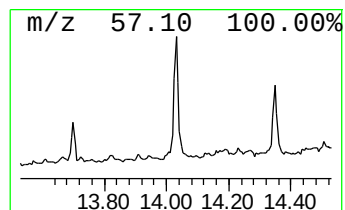
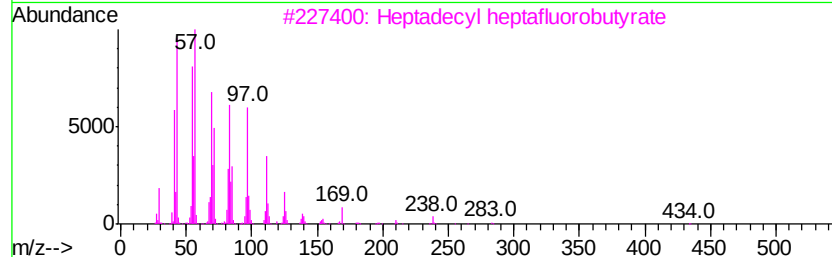
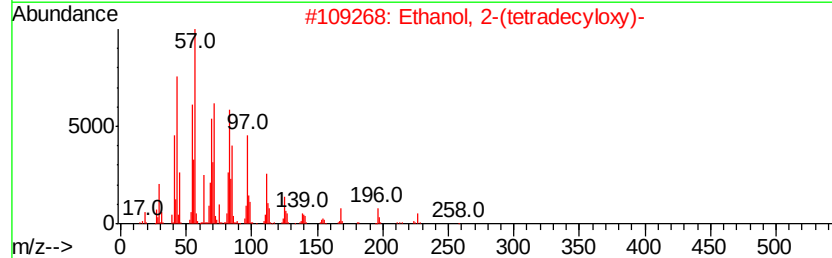
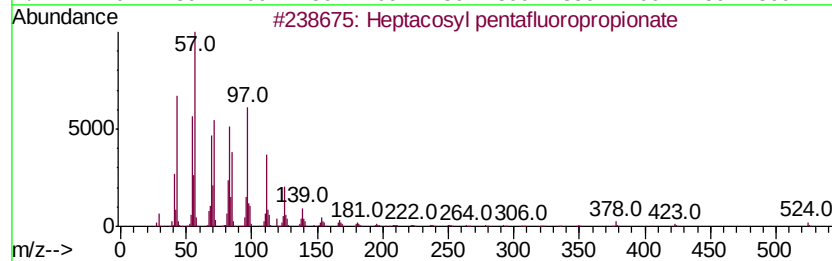
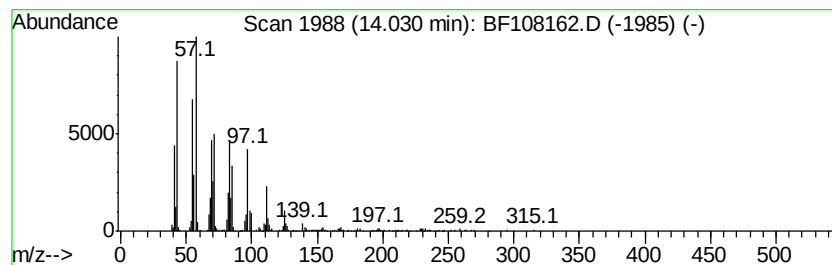
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Heptacosyl pentafluoropropi... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.03	7.04 ng	380786	Chrysene-d12	14.22

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptacosyl pentafluoropropionate	542	C30H55F5O2	1000351-81-6	91
2		Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
3		Heptadecyl heptafluorobutyrte	452	C21H35F7O2	959085-66-6	91
4		Octacosyl heptafluorobutyrte	606	C32H57F7O2	1000351-83-6	91
5		Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081518\
Data File : BF108162.D
Acq On : 15 Aug 2018 13:37
Operator : JU/SJ
Sample : J4447-36
Misc :
ALS Vial : 5 Sample Multiplier: 1

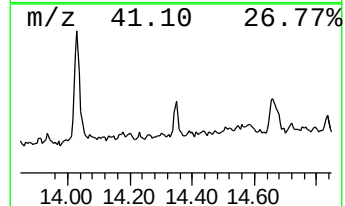
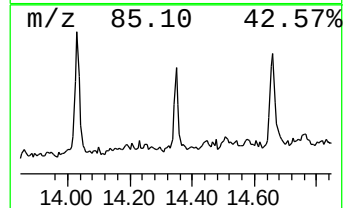
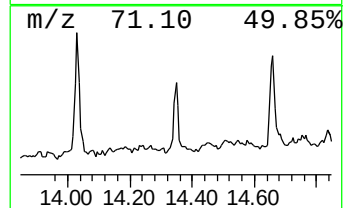
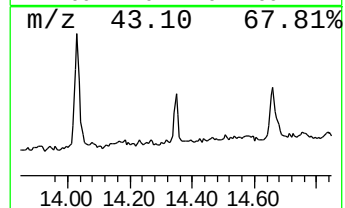
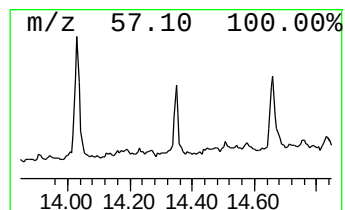
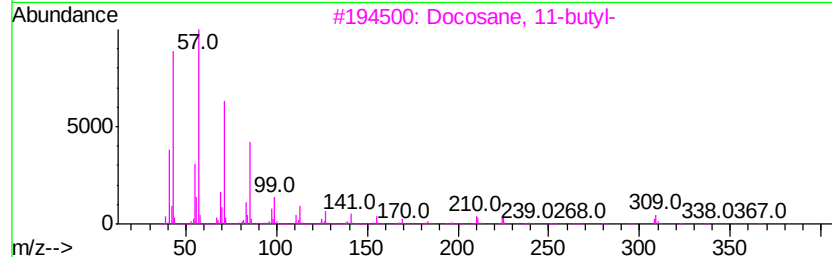
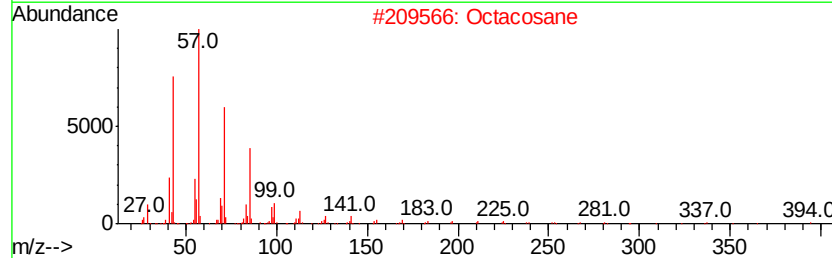
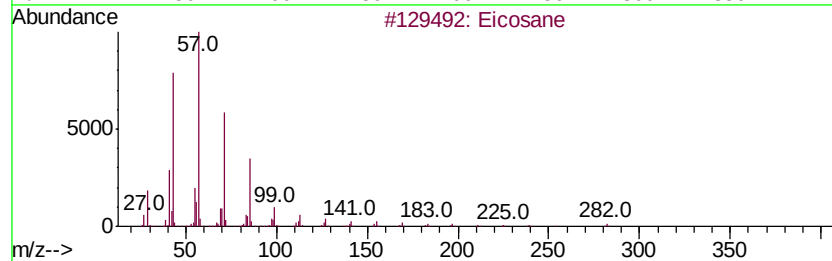
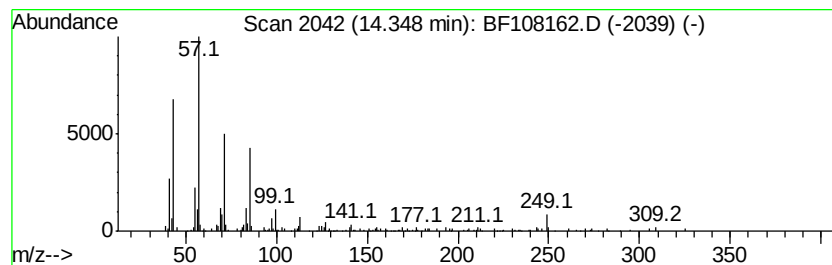
Instrument :
BNA_F
ClientSampleId :
SP-1-10

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Eicosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.35	2.20 ng	119033	Chrysene-d12	14.22
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Eicosane		282 C20H42	000112-95-8 93
2	Octacosane		394 C28H58	000630-02-4 87
3	Docosane, 11-butyl-		366 C26H54	013475-76-8 83
4	Tridecane, 1-iodo-		310 C13H27I	035599-77-0 80
5	Tridecane, 6-propyl-		226 C16H34	055045-10-8 80



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081518\
Data File : BF108162.D
Acq On : 15 Aug 2018 13:37
Operator : JU/SJ
Sample : J4447-36
Misc :
ALS Vial : 5 Sample Multiplier: 1

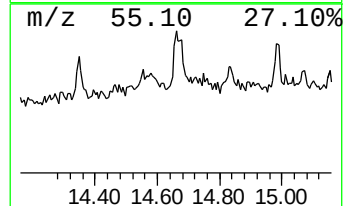
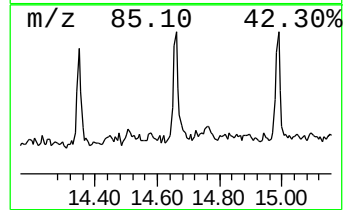
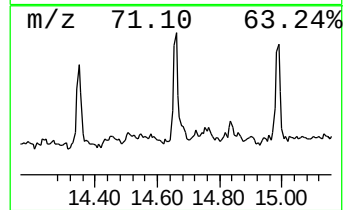
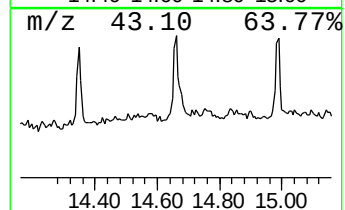
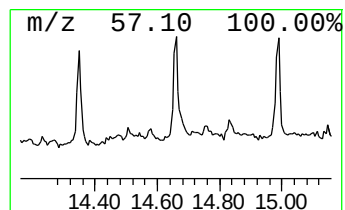
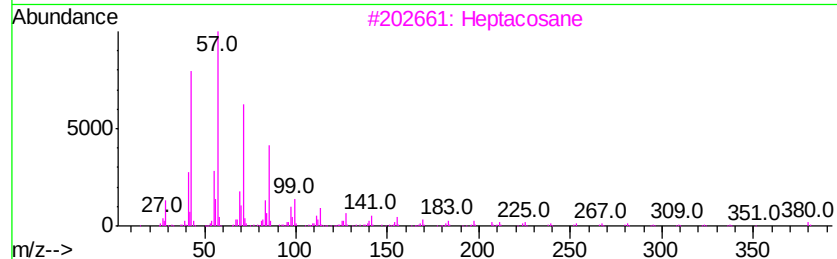
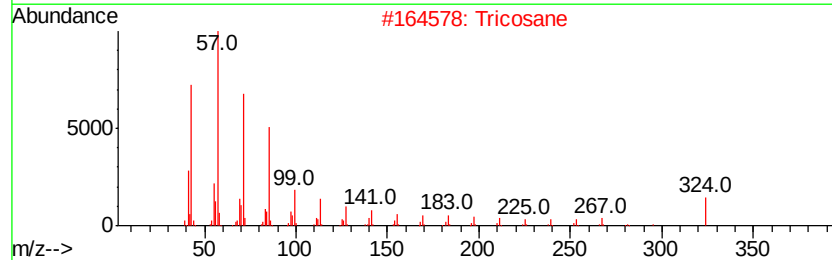
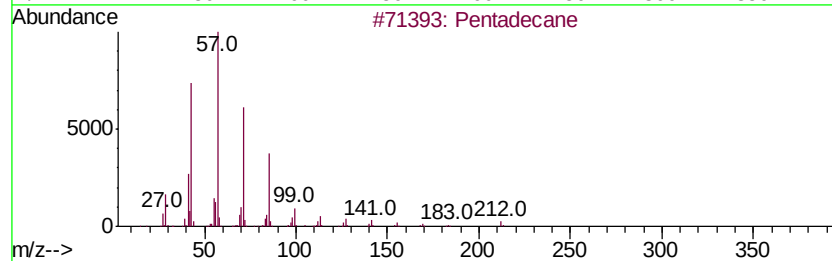
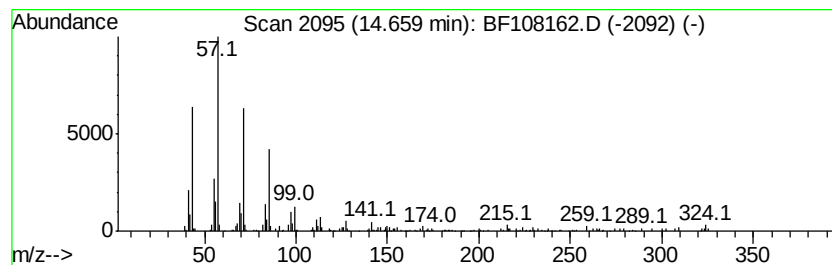
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ClientSampleId :
SP-1-10

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Pentadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.66	3.74 ng	202436	Chrysene-d12	14.22
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Pentadecane	212 C15H32	000629-62-9	94
2	Tricosane	324 C23H48	000638-67-5	91
3	Heptacosane	380 C27H56	000593-49-7	90
4	Hexadecane, 2,6,10,14-tetramethyl-	282 C20H42	000638-36-8	90
5	Hexacosane	366 C26H54	000630-01-3	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081518\
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Acq On : 15 Aug 2018 13:37
Operator : JU/SJ
Sample : J4447-36
Misc :
ALS Vial : 5 Sample Multiplier: 1

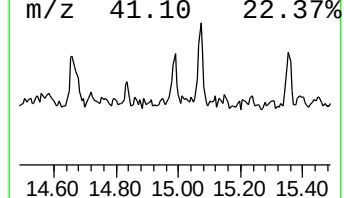
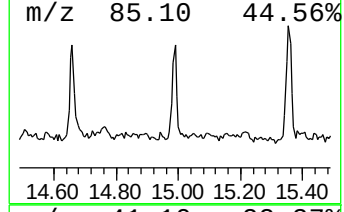
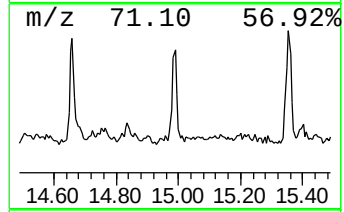
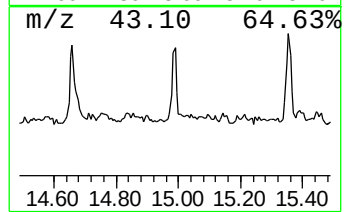
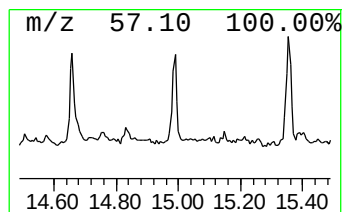
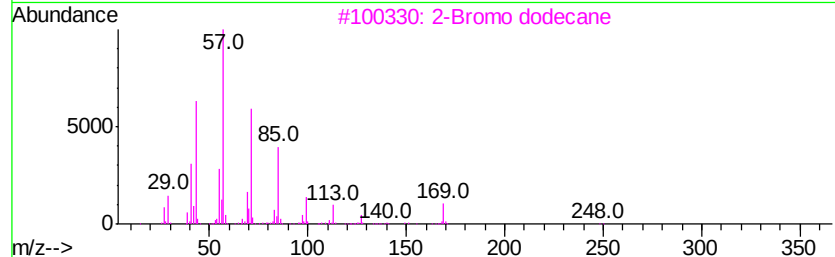
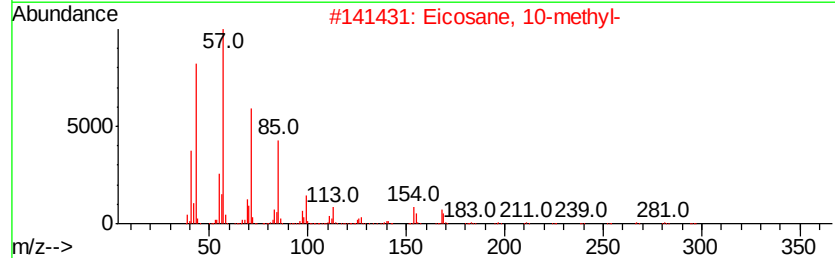
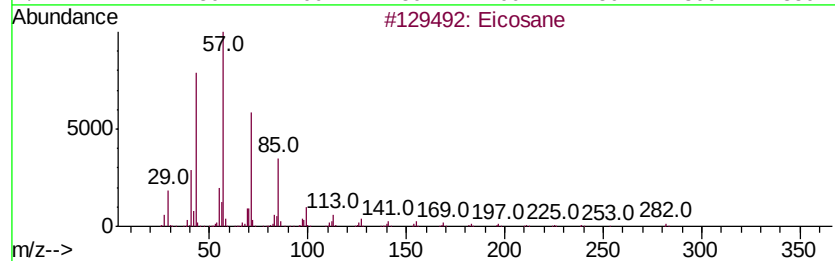
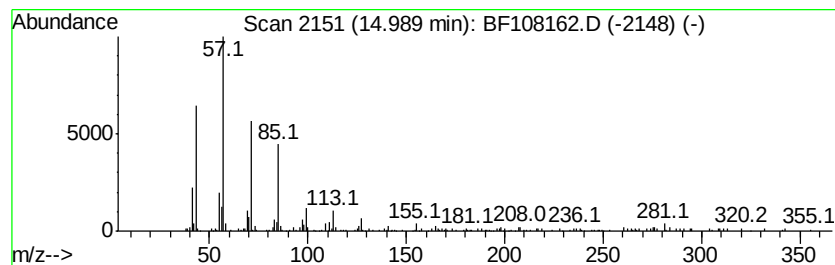
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Eicosane, 10-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.99	2.29 ng	123683	Chrysene-d12	14.22
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Eicosane		282 C20H42	000112-95-8 87
2	Eicosane, 10-methyl-		296 C21H44	054833-23-7 83
3	2-Bromo dodecane		248 C12H25Br	013187-99-0 80
4	Hentriacontane		437 C31H64	000630-04-6 80
5	Tridecane, 1-iodo-		310 C13H27I	035599-77-0 80



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081518\
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Misc :
ALS Vial : 5 Sample Multiplier: 1

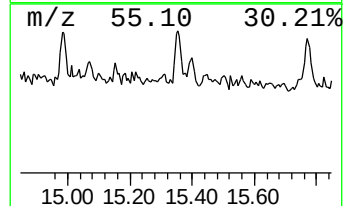
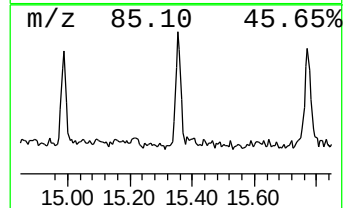
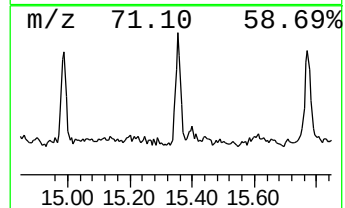
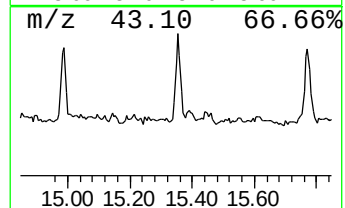
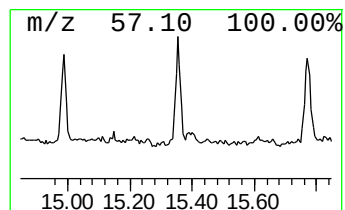
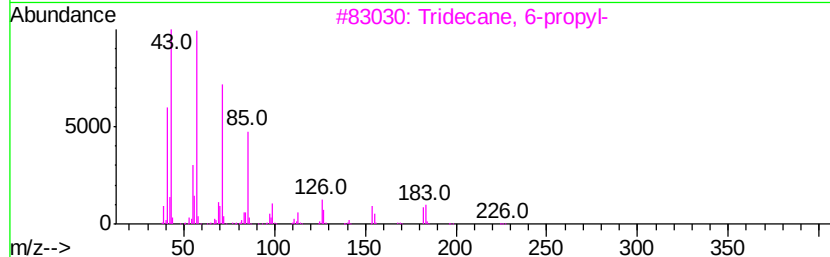
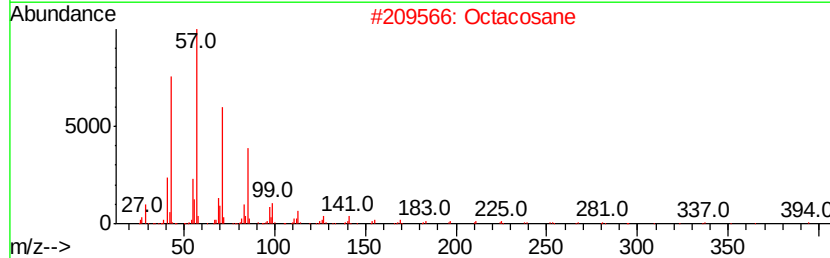
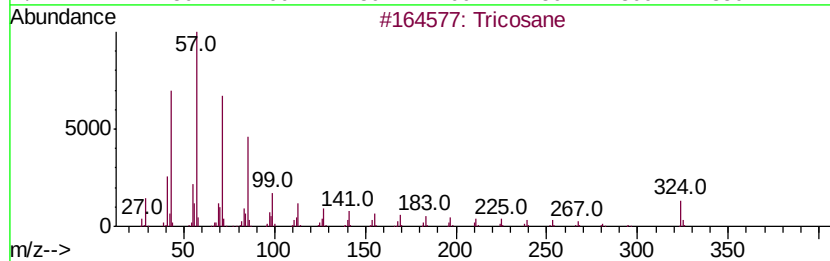
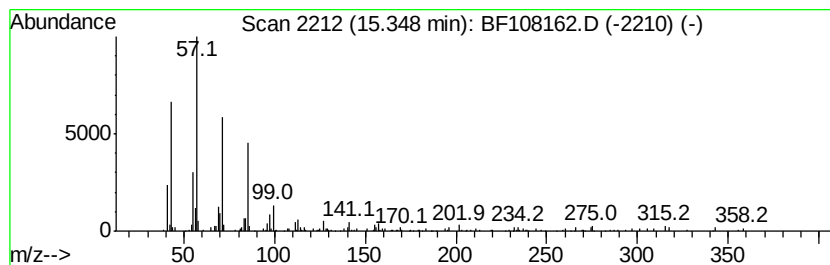
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Tricosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.35	2.31 ng	160666	Perylene-d12	15.78
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Tricosane	324 C23H48	000638-67-5	87
2	Octacosane	394 C28H58	000630-02-4	87
3	Tridecane, 6-propyl-	226 C16H34	055045-10-8	81
4	Docosane	310 C22H46	000629-97-0	80
5	5-Ethyl-5-methylnonadecane	310 C22H46	1000360-42-7	80



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081518\
Data File : BF108162.D
Acq On : 15 Aug 2018 13:37
Operator : JU/SJ
Sample : J4447-36
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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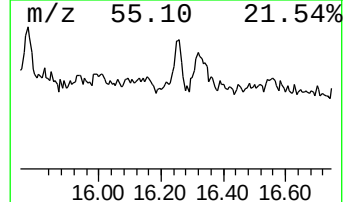
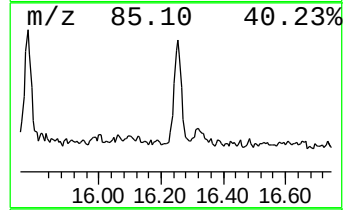
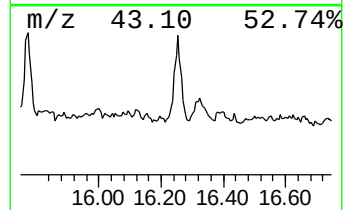
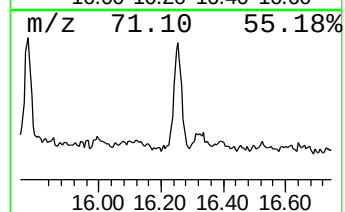
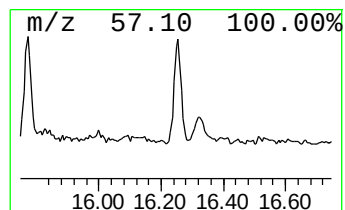
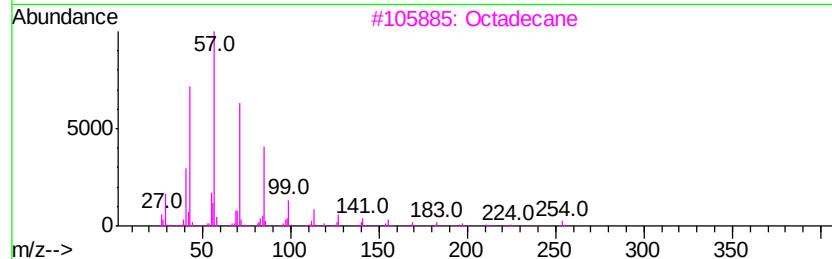
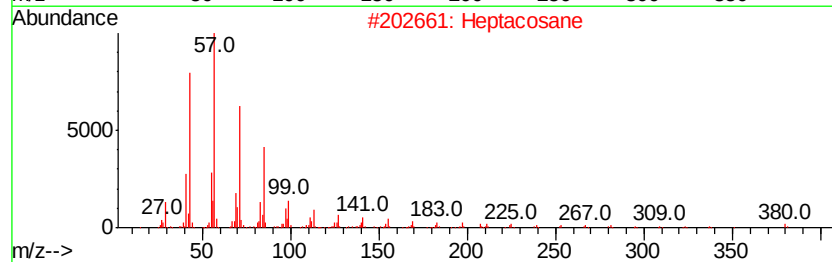
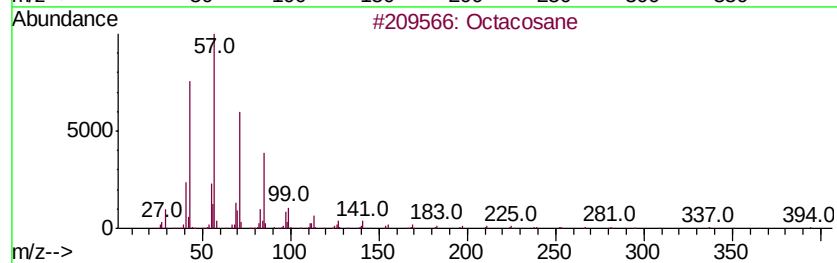
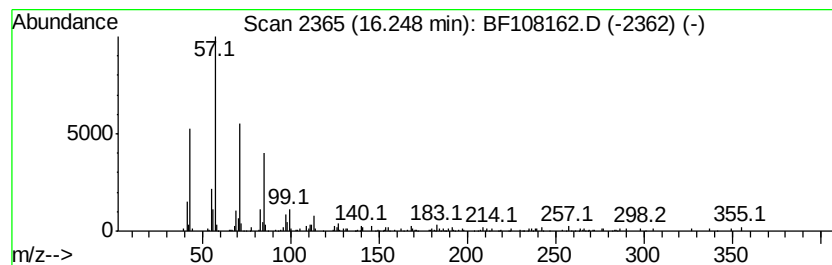
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Octacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.25	3.01 ng	208600	Perylene-d12	15.78

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	87
2		Heptacosane	380	C27H56	000593-49-7	83
3		Octadecane	254	C18H38	000593-45-3	83
4		Tetracosane	338	C24H50	000646-31-1	83
5		Hexacosane	366	C26H54	000630-01-3	81



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081518\
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Sample : J4447-36
Misc :
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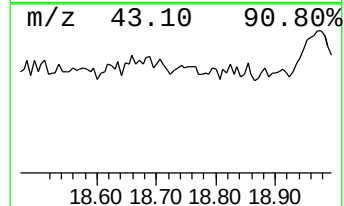
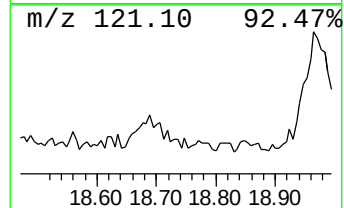
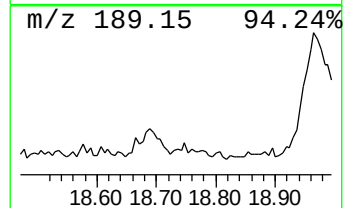
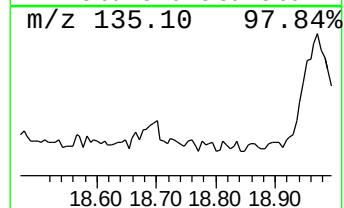
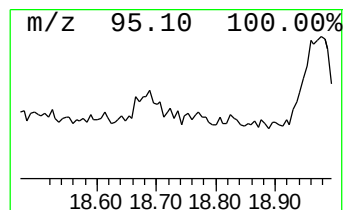
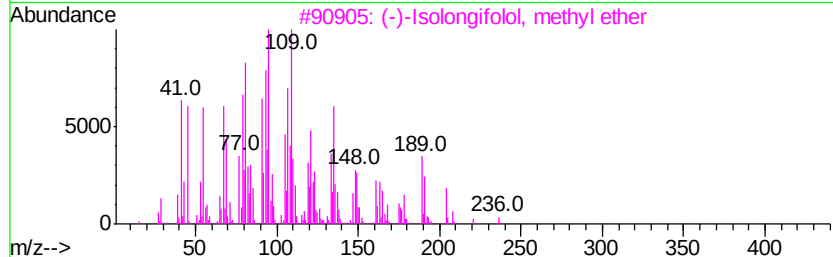
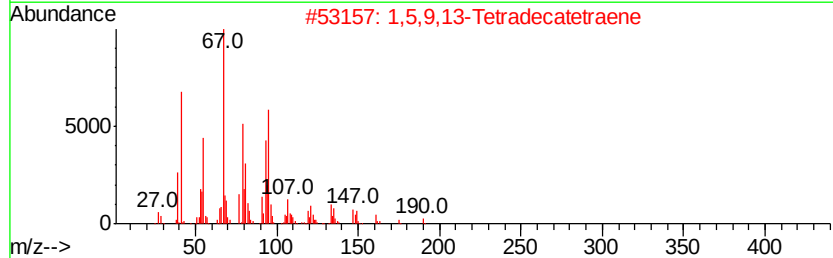
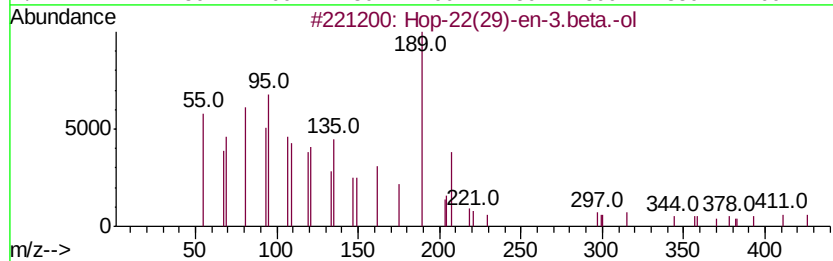
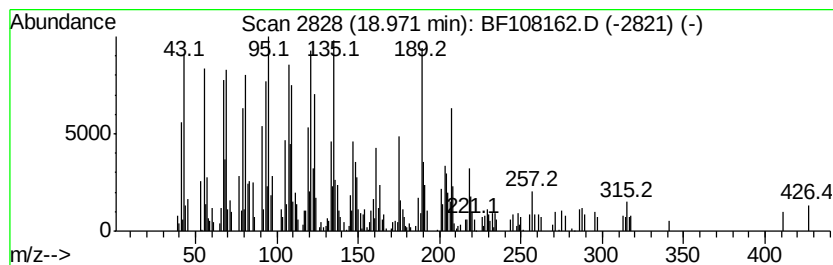
Instrument :
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 Hop-22(29)-en-3.beta.-ol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.97	3.12 ng	216736	Perylene-d12	15.78	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hop-22(29)-en-3.beta.-ol	426	C30H50O	058801-23-3	64
2	1,5,9,13-Tetradecatetraene	190	C14H22	051487-38-8	56
3	(-)-Isolongifolol, methyl ether	236	C16H28O	1000333-80-8	55
4	Cyclopropa[1,4]naphthalen-2(4aH)-o...	204	C14H20O	004677-90-1	55
5	Guaia-9,11-diene	204	C15H24	1000374-19-8	52



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF081518\
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Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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2-Pentanone, 4-hy...	5.27	16.5	ng	904680	1	7.02	1099120	20.0
unknown6.79	6.79	79.0	ng	4340930	1	7.02	1099120	20.0
Dodecane, 2,7,10-...	10.96	2.6	ng	165144	4	11.56	1248960	20.0
Heptacosyl penta...	14.03	7.0	ng	380786	5	14.22	1082140	20.0
Eicosane	14.35	2.2	ng	119033	5	14.22	1082140	20.0
Pentadecane	14.66	3.7	ng	202436	5	14.22	1082140	20.0
Eicosane, 10-methyl-	14.99	2.3	ng	123683	5	14.22	1082140	20.0
Tricosane	15.35	2.3	ng	160666	6	15.78	1388290	20.0
Octacosane	16.25	3.0	ng	208600	6	15.78	1388290	20.0
Hop-22(29)-en-3.b...	18.97	3.1	ng	216736	6	15.78	1388290	20.0