

Data Path : Z:\HPCHEM1\BNA F\DATA\BF082517\
 Data File : BF098044.D
 Acq On : 25 Aug 2017 21:42
 Operator : SJ/JU
 Sample : I4956-01
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 FK-GF-02-010-A

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:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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	4.940	481	485	496	rVB	204098	289745	8.62%	0.995%
2	5.351	549	555	558	rBV	2950609	3118400	92.78%	10.707%
3	6.381	719	730	736	rBV	2733493	3361215	100.00%	11.541%
4	6.510	747	752	755	rBV	3168879	3065634	91.21%	10.526%
5	6.740	787	791	794	rBV	930342	746522	22.21%	2.563%
6	6.898	811	818	821	rBV	2442789	2371927	70.57%	8.144%
7	7.304	882	887	890	rBV	2019360	1954191	58.14%	6.710%
8	7.387	898	901	907	rVB2	26939	35171	1.05%	0.121%
9	8.022	1005	1009	1012	rBV	1084284	893957	26.60%	3.069%
10	9.098	1187	1192	1195	rBV	3236335	2985864	88.83%	10.252%
11	9.492	1255	1259	1263	rBV	273575	224363	6.68%	0.770%
12	9.716	1293	1297	1301	rVB2	45596	58544	1.74%	0.201%
13	9.775	1301	1307	1310	rBV	912296	825670	24.56%	2.835%
14	10.210	1378	1381	1384	rVB	52159	38232	1.14%	0.131%
15	10.557	1436	1440	1444	rBV	1408181	1370244	40.77%	4.705%
16	10.669	1455	1459	1468	rBV	456278	439562	13.08%	1.509%
17	11.251	1555	1558	1561	rBV	753802	684345	20.36%	2.350%
18	11.275	1561	1562	1565	rVV	202081	122348	3.64%	0.420%
19	11.328	1565	1571	1574	rVB	65604	53699	1.60%	0.184%
20	11.486	1592	1598	1606	rBV2	69500	83123	2.47%	0.285%
21	11.863	1659	1662	1665	rBV	41269	42700	1.27%	0.147%
22	12.304	1733	1737	1742	rBV	321554	330089	9.82%	1.133%
23	12.357	1744	1746	1749	rVB2	48134	37688	1.12%	0.129%
24	12.463	1758	1764	1767	rBV	330941	302040	8.99%	1.037%
25	12.686	1796	1802	1805	rBV	288548	309335	9.20%	1.062%
26	12.839	1824	1828	1831	rBV	2159517	1925134	57.27%	6.610%
27	13.016	1856	1858	1861	rVB	42743	35188	1.05%	0.121%
28	13.051	1861	1864	1867	rBV	47841	53566	1.59%	0.184%
29	13.116	1872	1875	1879	rBV2	31351	38686	1.15%	0.133%
30	13.286	1901	1904	1908	rVB	100844	88754	2.64%	0.305%
31	13.633	1959	1963	1966	rBV2	26990	38267	1.14%	0.131%
32	13.733	1977	1980	1986	rBV3	119535	151637	4.51%	0.521%
33	13.886	2000	2006	2008	rBV2	760720	907088	26.99%	3.115%
34	13.910	2008	2010	2012	rVB	133161	102669	3.05%	0.353%

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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:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.651	2132	2136	2143	rBV	629708	722284	21.49%	2.480%
36	14.733	2147	2150	2155	rVB	85938	97288	2.89%	0.334%
37	14.898	2174	2178	2181	rBV	119098	176793	5.26%	0.607%
38	15.180	2223	2226	2230	rVB	69373	84097	2.50%	0.289%
39	15.239	2233	2236	2240	rBV	96442	110774	3.30%	0.380%
40	15.304	2242	2247	2250	rBV	486098	571806	17.01%	1.963%
41	15.751	2320	2323	2328	rBV2	60461	93322	2.78%	0.320%
42	16.227	2401	2404	2408	rVB3	57565	79543	2.37%	0.273%
43	16.780	2494	2498	2505	rBV2	54915	103169	3.07%	0.354%

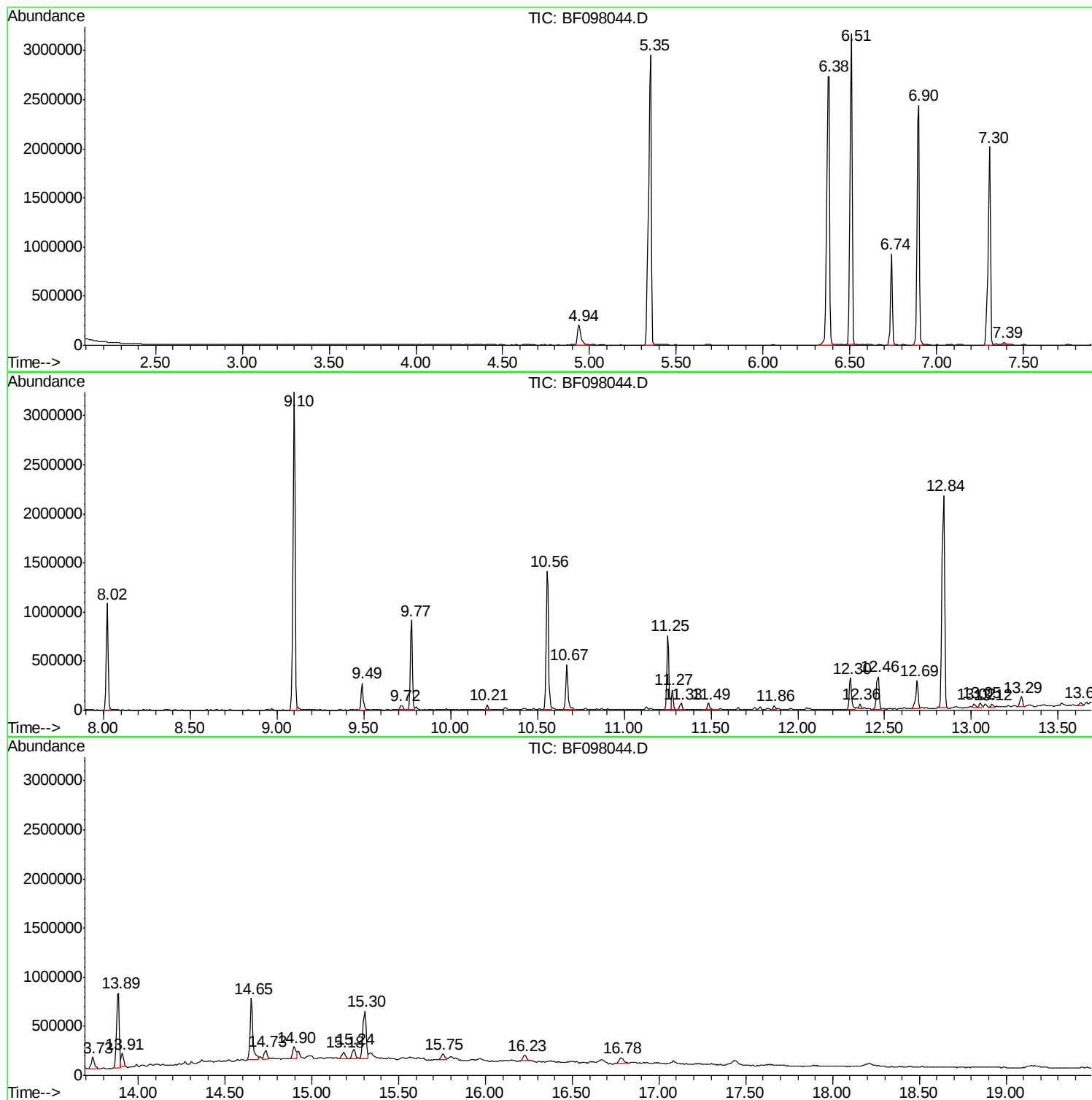
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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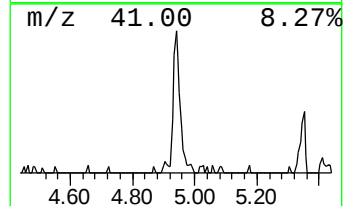
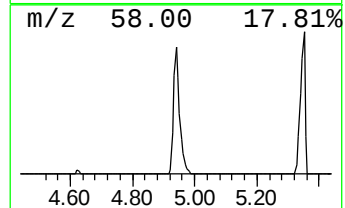
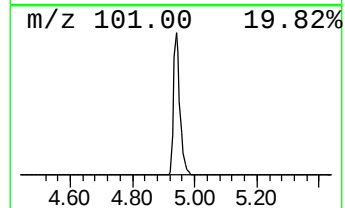
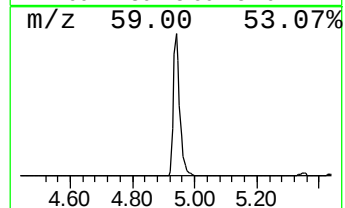
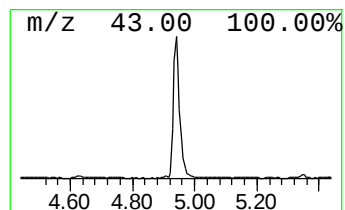
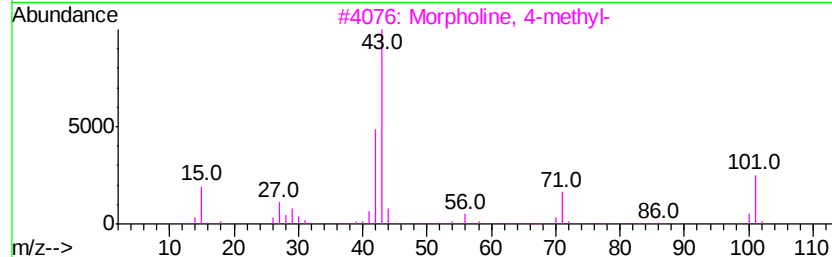
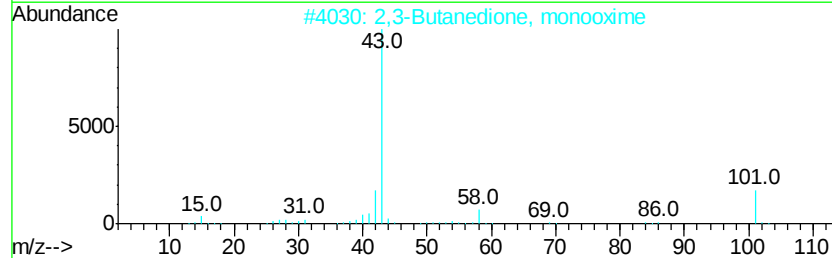
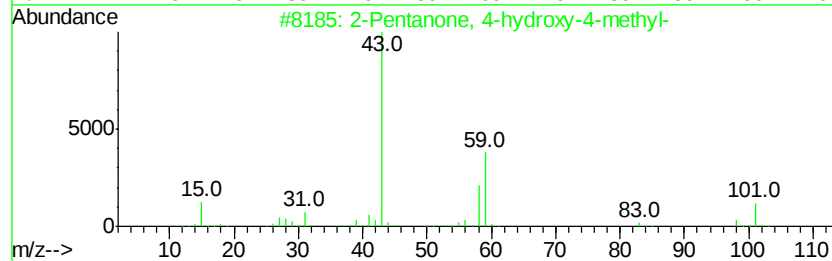
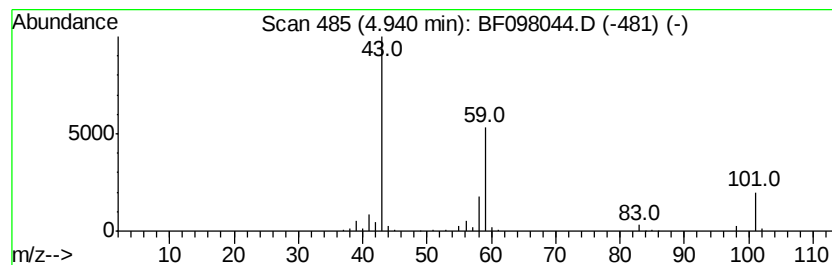
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.94	7.76 ng	289745	1,4-Dichlorobenzene-d4	6.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4		Butane	58	C4H10	000106-97-8	9
5		5-Hexen-2-one	98	C6H10O	000109-49-9	9



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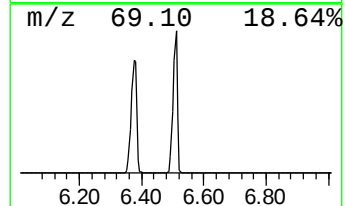
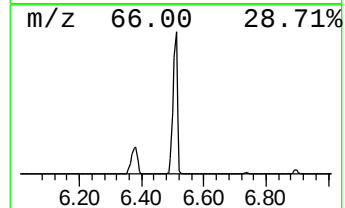
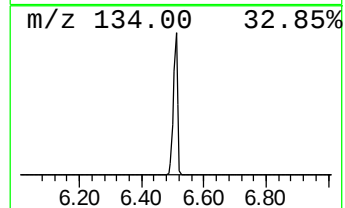
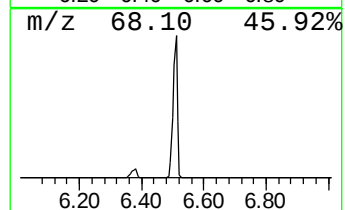
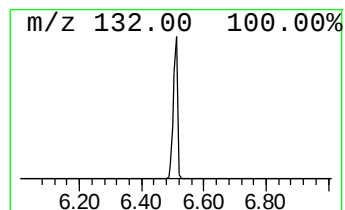
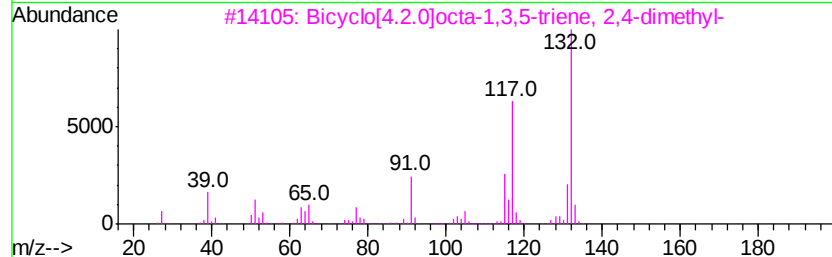
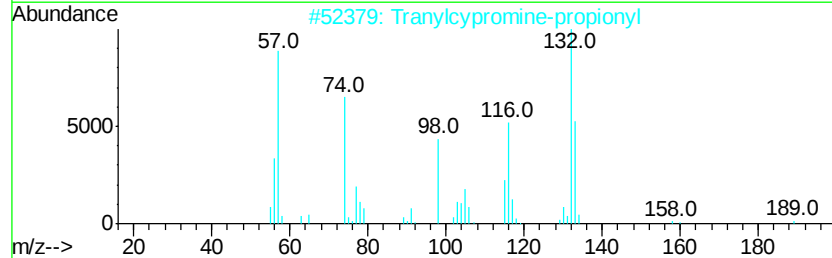
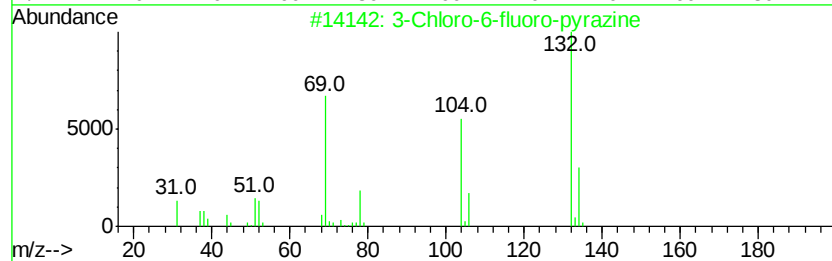
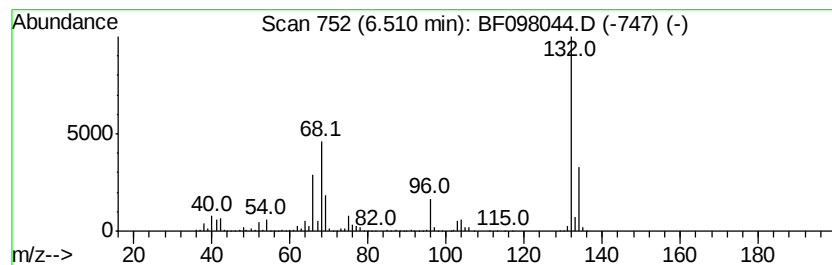
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.51 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.51	82.13 ng	3065630	1,4-Dichlorobenzene-d4	6.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
5		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9



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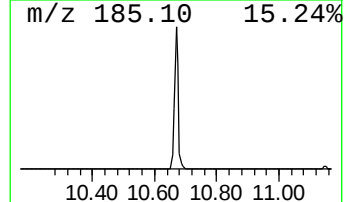
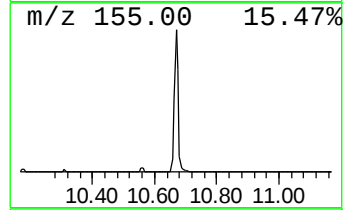
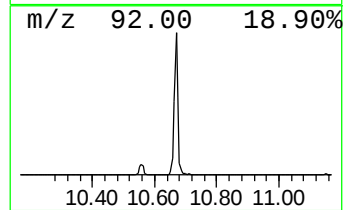
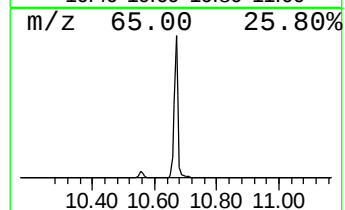
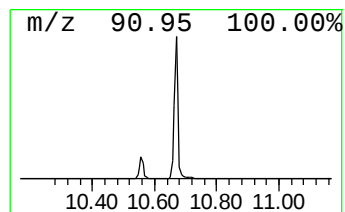
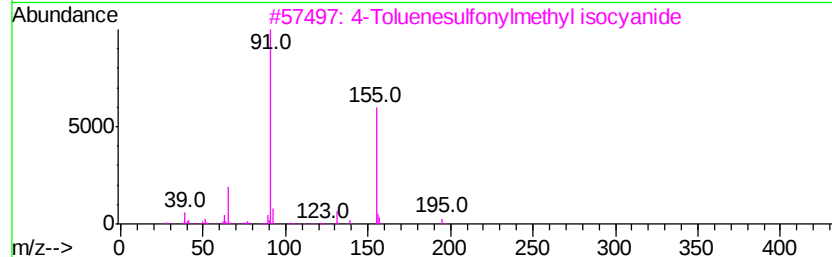
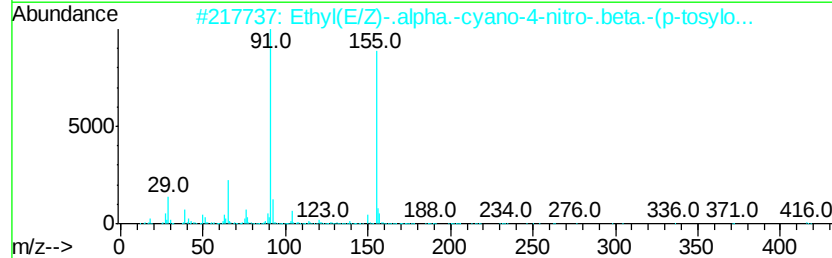
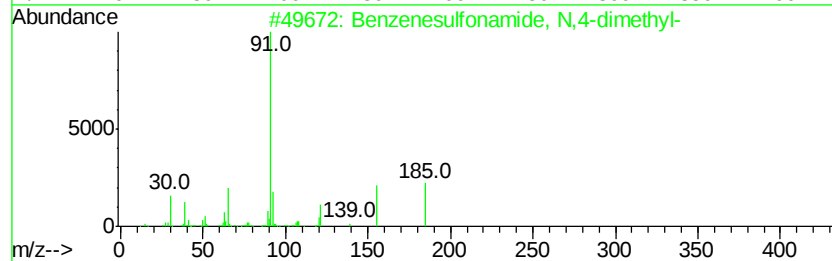
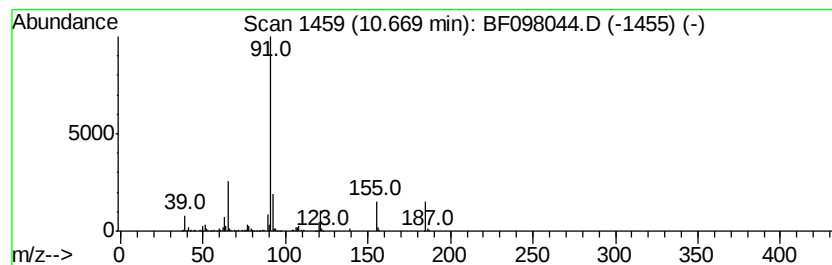
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Benzenesulfonamide, N,4-dim... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.67	12.85 ng	439562	Phenanthrene-d10	11.25

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzenesulfonamide, N,4-dimethyl-	185	C8H11NO2S	000640-61-9	94
2		Ethyl(E/Z)-.alpha.-cyano-4-nitro...	416	C19H16N2O7S	1000287-26-8	53
3		4-Toluenesulfonylmethyl isocyanide	195	C9H9NO2S	036635-61-7	50
4		(O-p-Tosylisonitroso)malononitrile	249	C10H7N3O3S	020893-01-0	50
5		Benzene, 1,1'-[sulfinylbis(methy...	230	C14H14OS	000621-08-9	47



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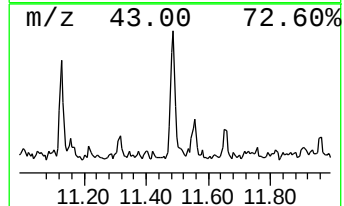
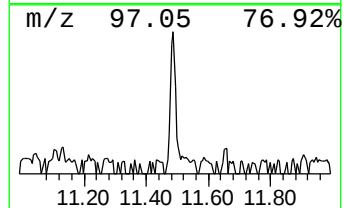
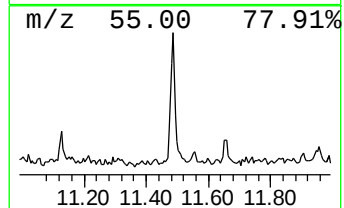
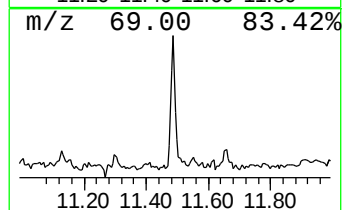
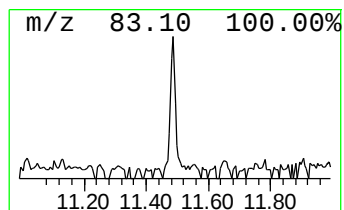
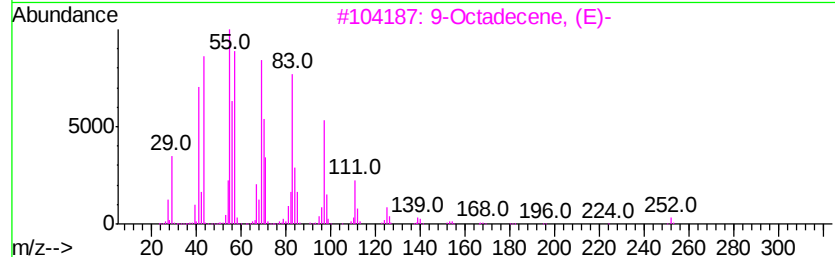
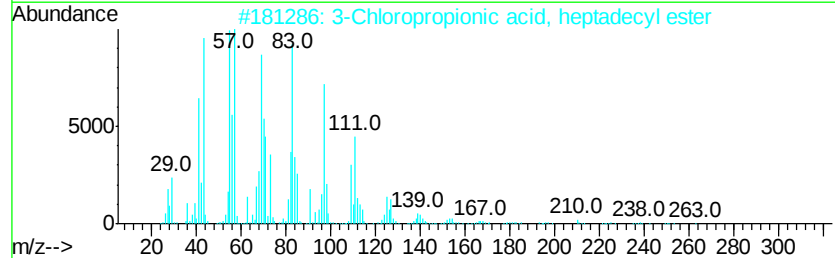
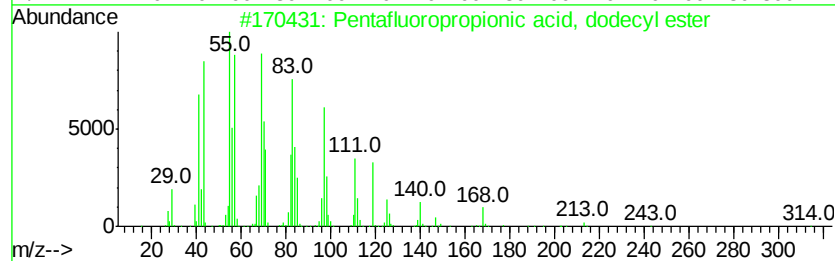
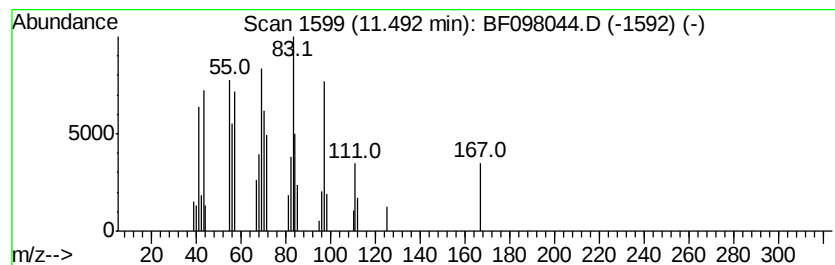
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Pentafluoropropionic acid, ... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.49	2.43 ng	83123	Phenanthrene-d10	11.25

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentafluoropropionic acid, dodec...	332	C15H25F5O2	006222-04-4	93
2		3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	90
3		9-Octadecene, (E)-	252	C18H36	007206-25-9	90
4		9-Eicosene, (E)-	280	C20H40	074685-29-3	87
5		4-Heptafluorobutyryloxyhexadecane	438	C20H33F7O2	1000282-97-2	87



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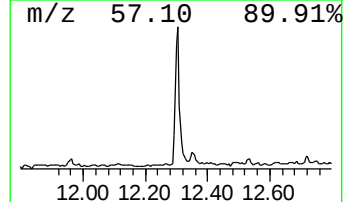
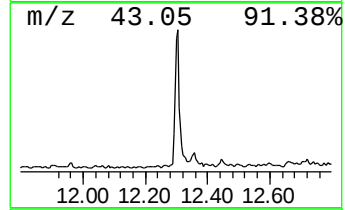
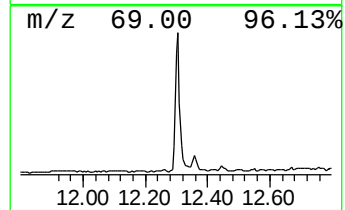
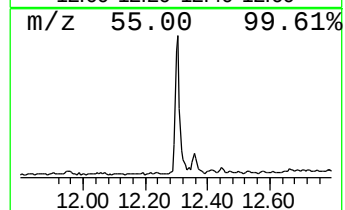
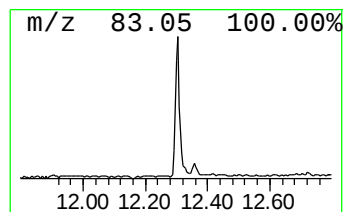
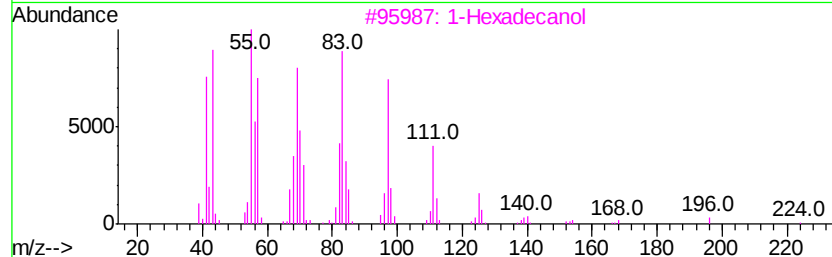
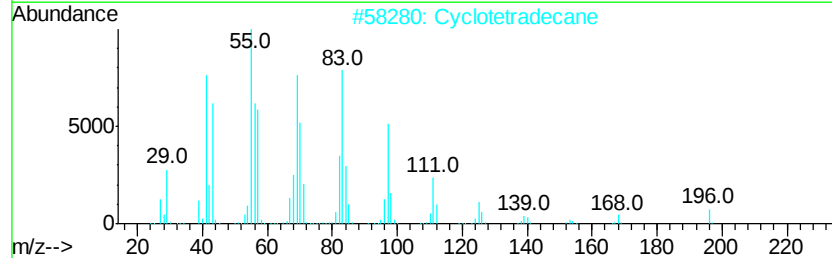
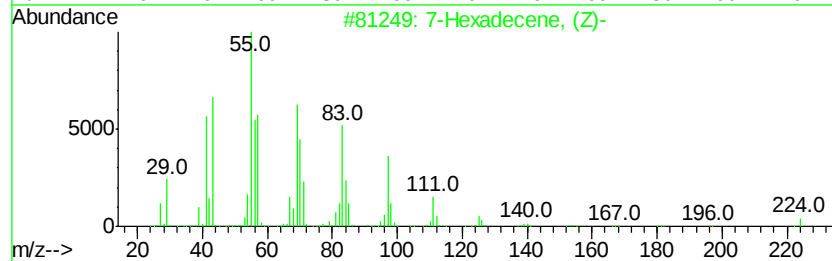
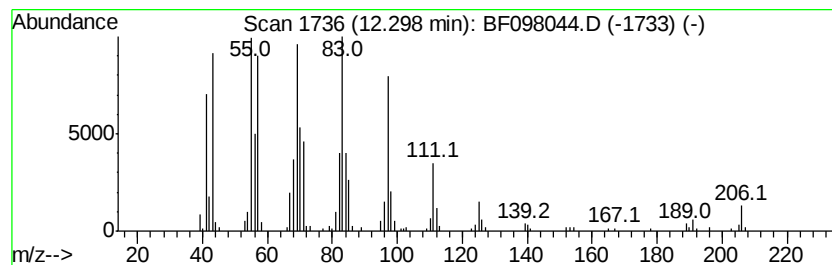
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 7-Hexadecene, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.30	9.65 ng	330089	Phenanthrene-d10	11.25	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7-Hexadecene, (Z)-	224	C16H32	035507-09-6	96
2	Cyclotetradecane	196	C14H28	000295-17-0	93
3	1-Hexadecanol	242	C16H34O	036653-82-4	93
4	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	91
5	1-Heneicosanol	312	C21H44O	015594-90-8	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082517\
Data File : BF098044.D
Acq On : 25 Aug 2017 21:42
Operator : SJ/JU
Sample : I4956-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

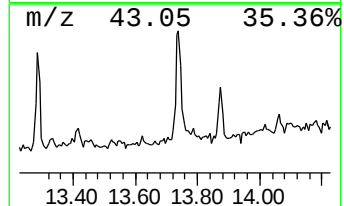
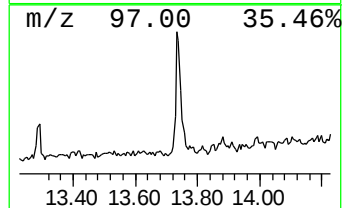
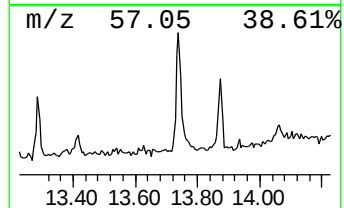
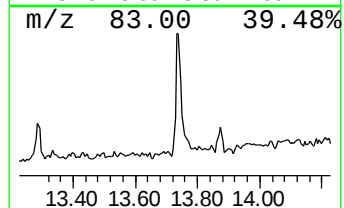
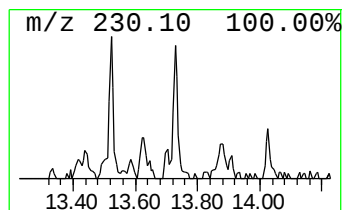
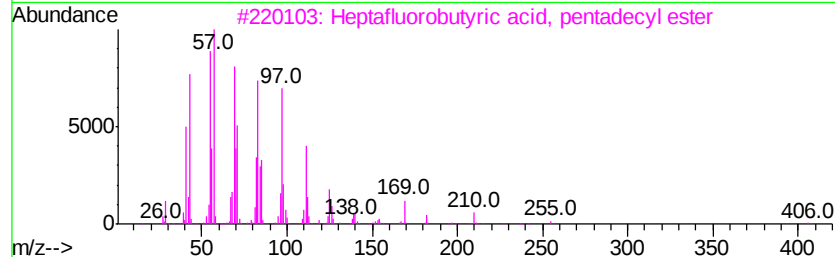
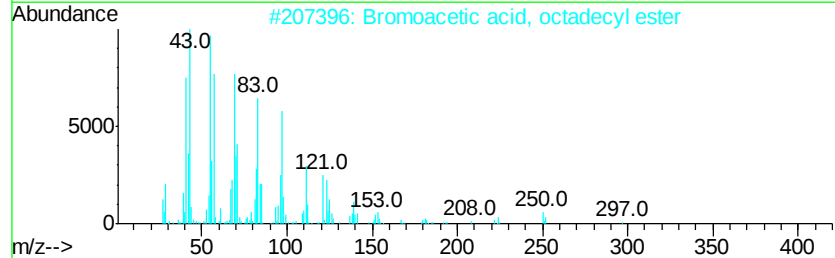
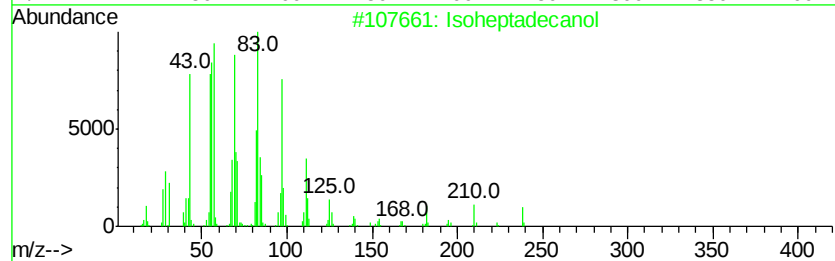
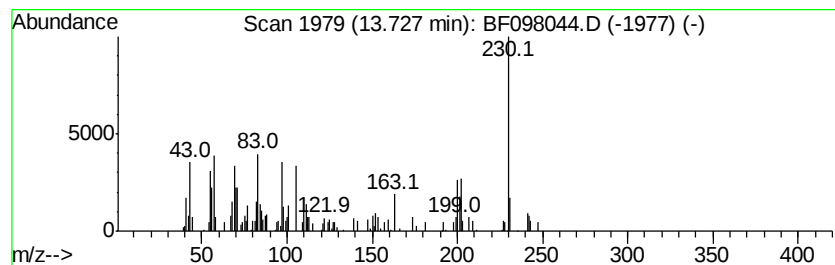
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Isoheptadecanol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.		
13.73	3.34 ng	151637	Chrysene-d12	13.89		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Isoheptadecanol	256	C17H36O	057289-07-3	87
2		Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	87
3		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	86
4		n-Nonadecanol-1	284	C19H40O	001454-84-8	83
5		1-Hexadecanol	242	C16H34O	036653-82-4	83



Data Path : Z:\HPCHEM1\BNA F\DATA\BF082517\
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Acq On : 25 Aug 2017 21:42
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ClientSampleId :
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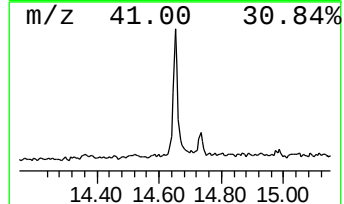
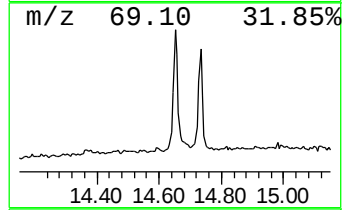
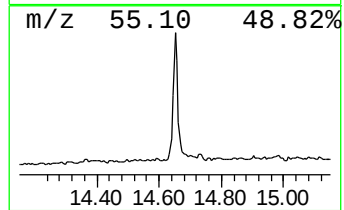
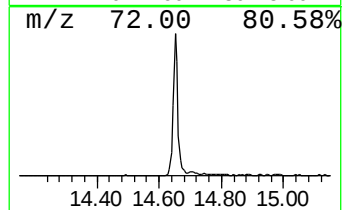
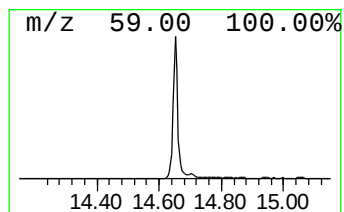
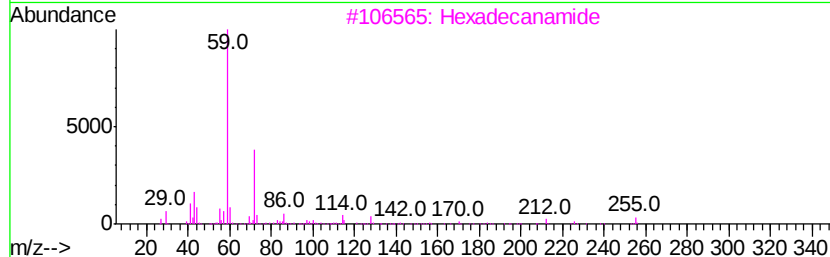
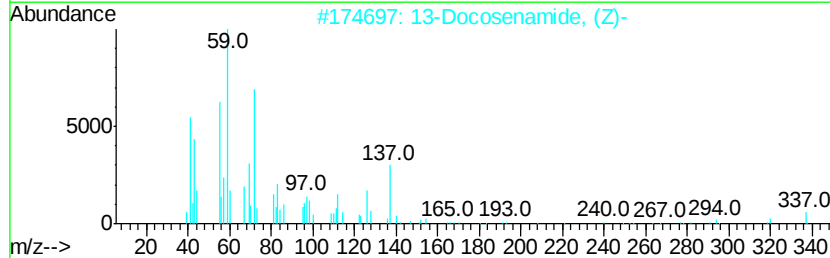
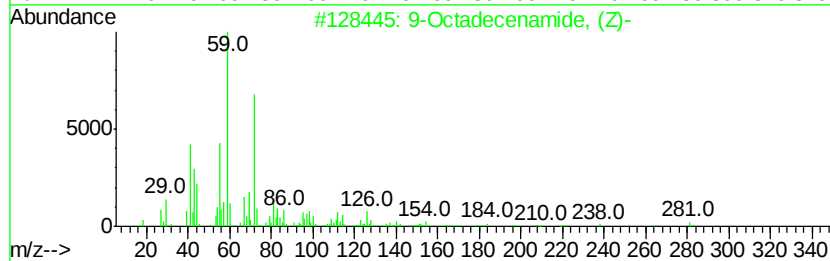
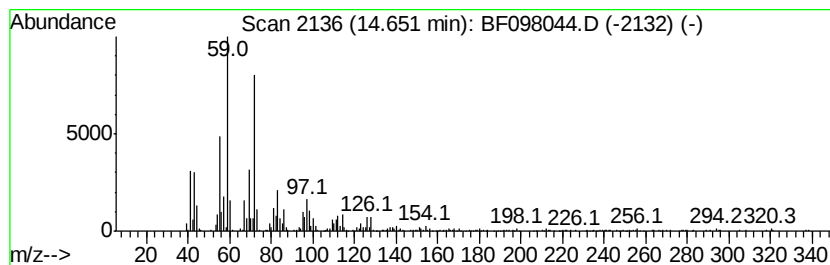
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 9-Octadecenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.65	25.26 ng	722284	Perylene-d12	15.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	86
2		13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	72
3		Hexadecanamide	255	C16H33NO	000629-54-9	59
4		1,1,2-Trimethyl-1-silacyclobutane	114	C6H14Si	030681-90-4	38
5		7-Nonenamide	155	C9H17NO	090949-53-4	35



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082517\
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Operator : SJ/JU
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Instrument :
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ClientSampleId :
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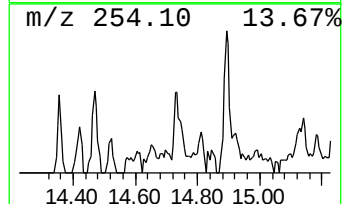
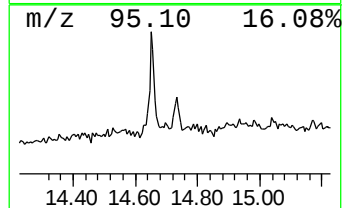
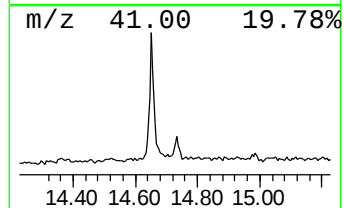
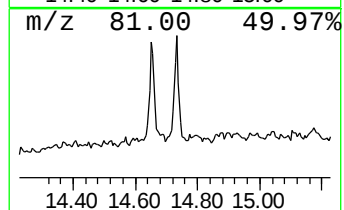
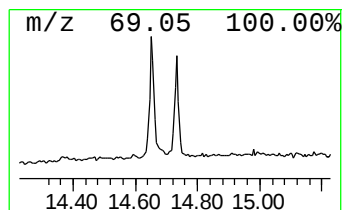
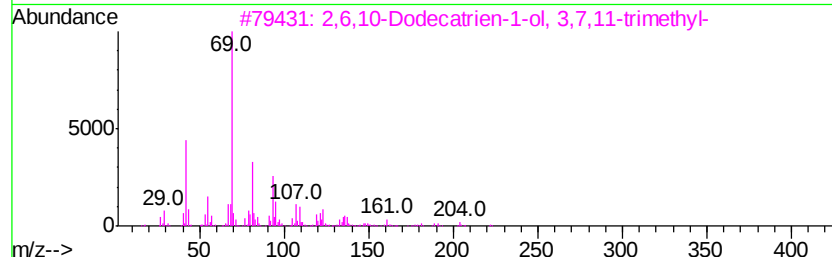
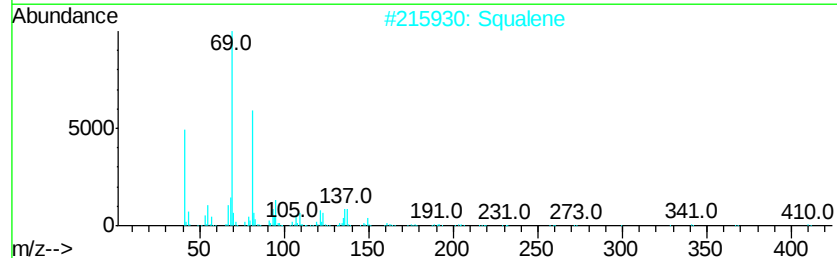
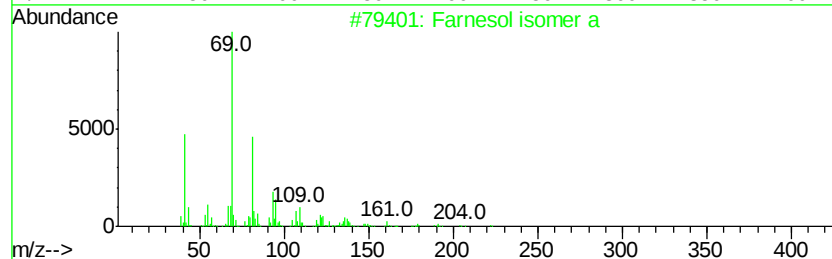
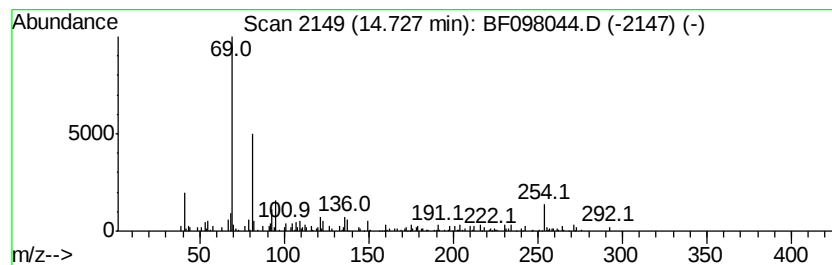
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Farnesol isomer a Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.73	3.40 ng	97288	Perylene-d12	15.30

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Farnesol isomer a	222	C15H26O	1000108-92-4	81	
2	Squalene	410	C30H50	000111-02-4	81	
3	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	72	
4	Supraene	410	C30H50	007683-64-9	72	
5	.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	64	



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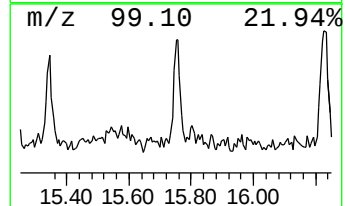
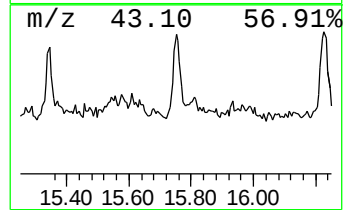
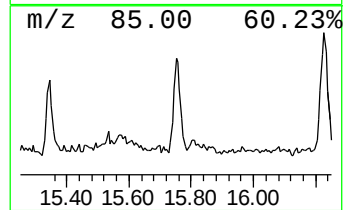
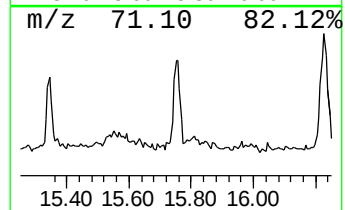
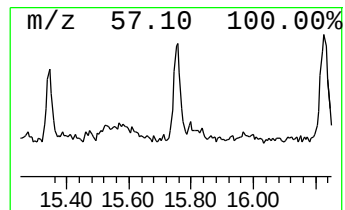
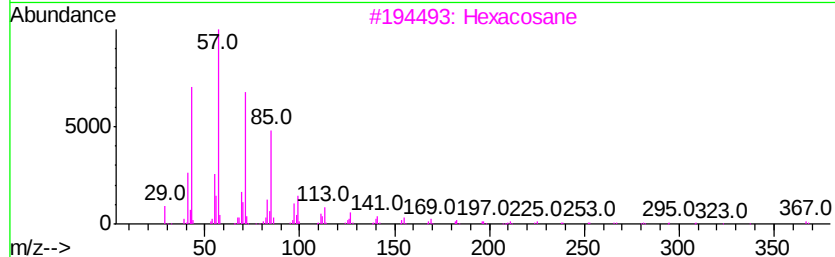
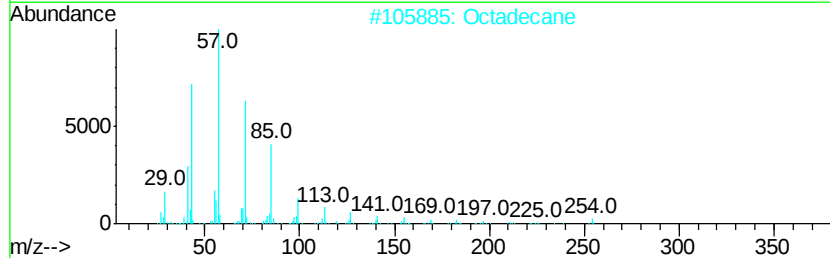
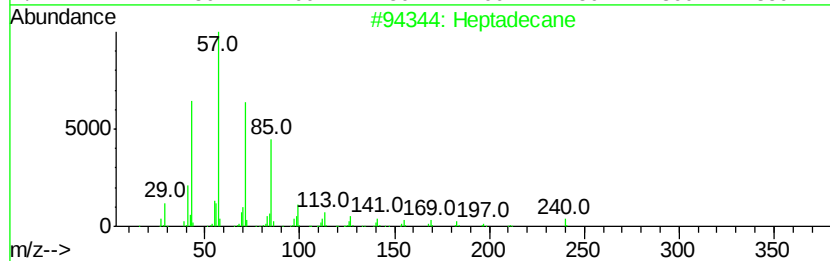
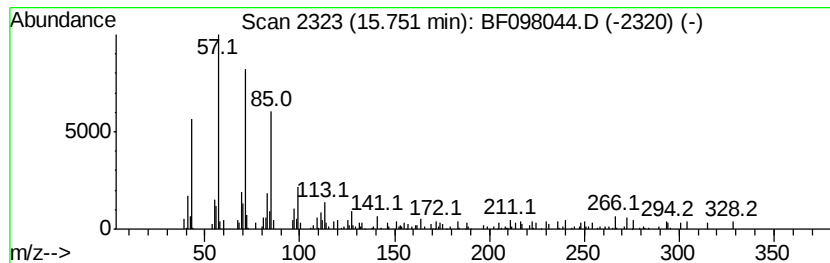
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Heptadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.75	3.26 ng	93322	Perylene-d12	15.30

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecane	240	C17H36	000629-78-7	94
2			Octadecane	254	C18H38	000593-45-3	91
3			Hexacosane	366	C26H54	000630-01-3	81
4			10-Methylnonadecane	282	C20H42	056862-62-5	74
5			Heneicosane	296	C21H44	000629-94-7	74



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082517\
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Acq On : 25 Aug 2017 21:42
Operator : SJ/JU
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ClientSampleId :
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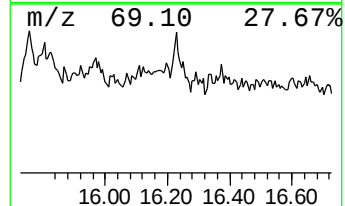
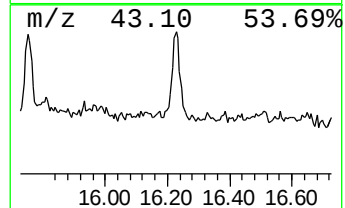
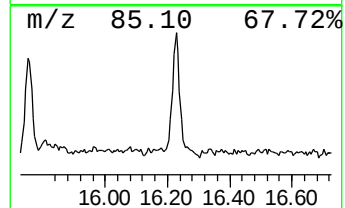
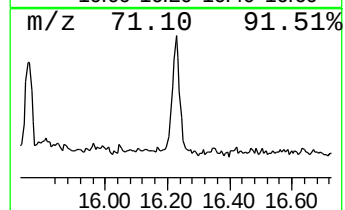
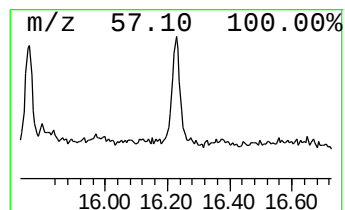
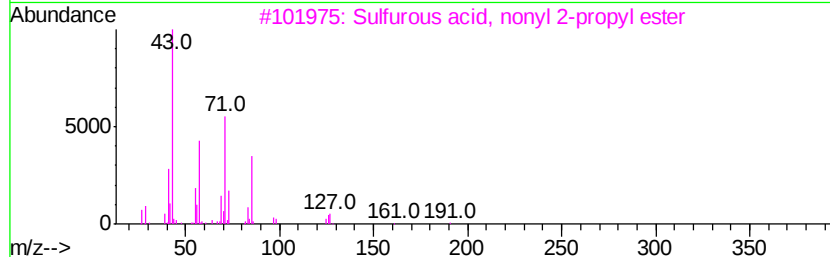
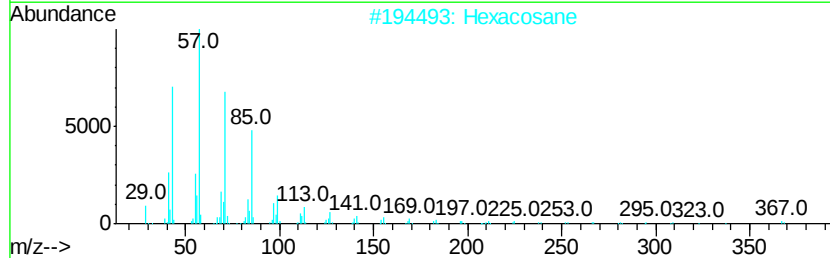
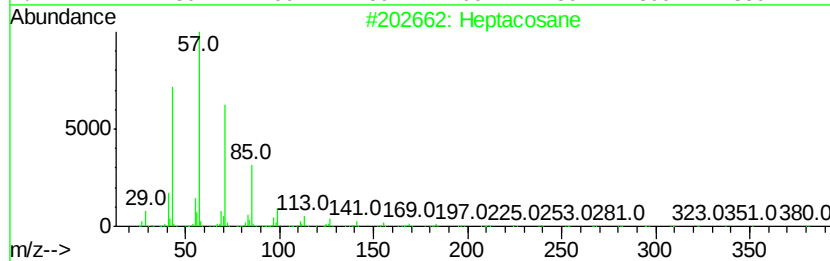
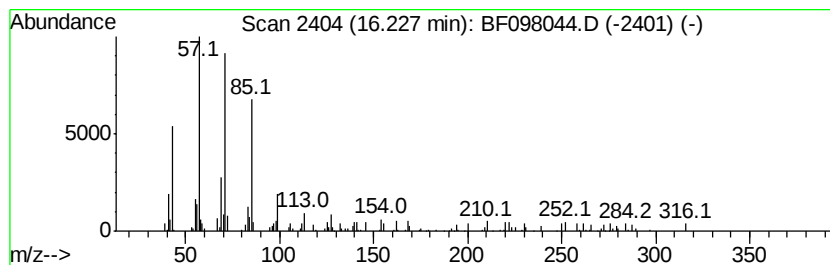
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Heptacosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.23	2.78 ng	79543	Perylene-d12	15.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptacosane	380	C27H56	000593-49-7	64
2		Hexacosane	366	C26H54	000630-01-3	64
3		Sulfurous acid, nonyl 2-propyl e...	250	C12H26O3S	1000309-12-0	64
4		Oxalic acid, 6-ethyloct-3-yl hep...	328	C19H36O4	1000309-34-5	59
5		Octadecane	254	C18H38	000593-45-3	59



Data Path : Z:\HPCHEM1\BNA F\DATA\BF082517\
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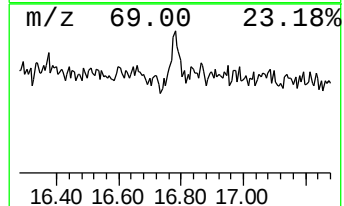
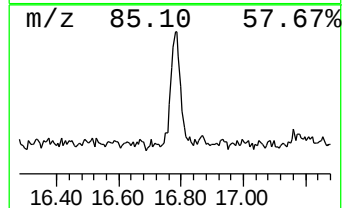
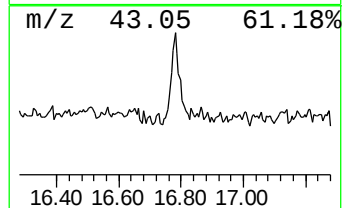
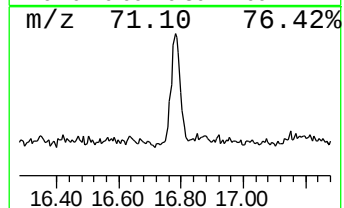
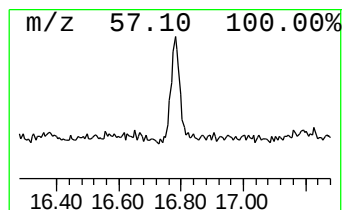
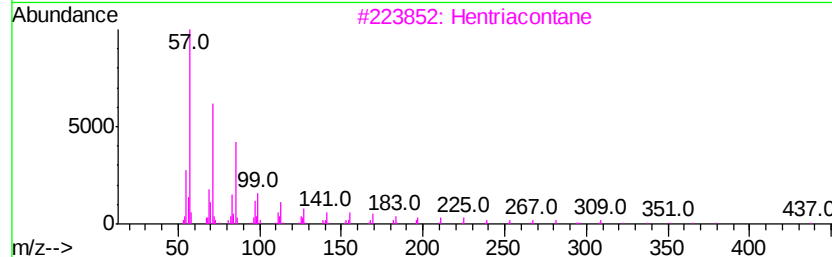
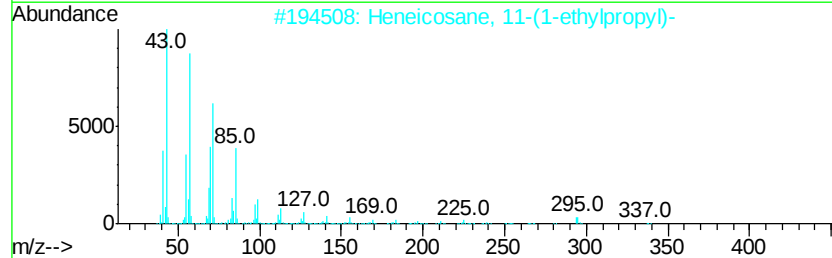
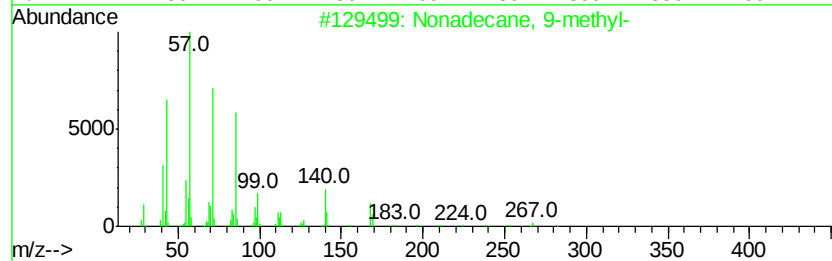
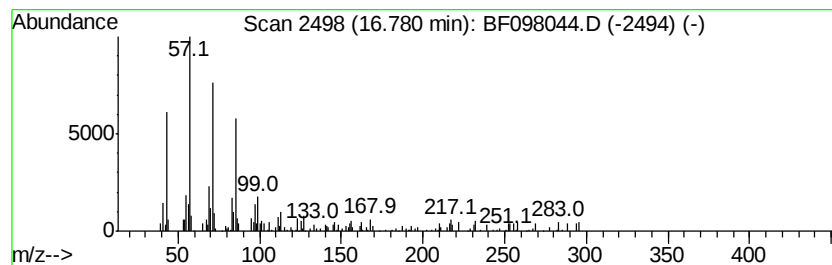
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Nonadecane, 9-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.78	3.61 ng	103169	Perylene-d12	15.30

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane, 9-methyl-	282	C20H42	013287-24-6	76
2			Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	74
3			Hentriacontane	437	C31H64	000630-04-6	68
4			2-methyloctacosane	408	C29H60	1000376-72-8	68
5			Octadecane	254	C18H38	000593-45-3	64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082517\
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 ALS Vial : 14 Sample Multiplier: 1

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 ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
 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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unknown6.51	6.51	82.1	ng	3065630	1	6.74	746522	20.0
Benzenesulfonamid...	10.67	12.9	ng	439562	4	11.25	684345	20.0
Pentafluoropropio...	11.49	2.4	ng	83123	4	11.25	684345	20.0
7-Hexadecene, (Z)-	12.30	9.7	ng	330089	4	11.25	684345	20.0
Isoheptadecanol	13.73	3.3	ng	151637	5	13.89	907088	20.0
9-Octadecenamide, ...	14.65	25.3	ng	722284	6	15.30	571806	20.0
Farnesol isomer a	14.73	3.4	ng	97288	6	15.30	571806	20.0
Heptadecane	15.75	3.3	ng	93322	6	15.30	571806	20.0
Heptacosane	16.23	2.8	ng	79543	6	15.30	571806	20.0
Nonadecane, 9-met...	16.78	3.6	ng	103169	6	15.30	571806	20.0