

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080817\
 Data File : BF097496.D
 Acq On : 9 Aug 2017 4:10
 Operator : SJ/JU
 Sample : I4604-02
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-2A-080217

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-BF072517.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	4.534	463	467	473	rBV	52539	88886	4.28%	0.515%
2	4.598	473	478	483	rVB5	12766	29196	1.41%	0.169%
3	4.810	510	514	523	rBV	31436	48435	2.33%	0.281%
4	5.004	543	547	572	rBV	995892	1435139	69.11%	8.312%
5	5.551	637	640	647	rBV	24601	25925	1.25%	0.150%
6	6.081	727	730	744	rVV	596086	815693	39.28%	4.724%
7	6.181	744	747	753	rVV	2056175	2032097	97.86%	11.769%
8	6.228	753	755	767	rVB	60298	80840	3.89%	0.468%
9	6.404	782	785	797	rBV	505173	505258	24.33%	2.926%
10	6.563	808	812	828	rVB	2036142	1973238	95.03%	11.429%
11	6.951	874	878	880	rBV2	52499	63035	3.04%	0.365%
12	6.981	880	883	897	rVB	1725982	1694764	81.62%	9.816%
13	7.192	915	919	921	rBV	43292	41640	2.01%	0.241%
14	7.216	921	923	928	rVB	34544	30182	1.45%	0.175%
15	7.369	947	949	955	rVB2	34894	40800	1.96%	0.236%
16	7.434	957	960	965	rBV2	77384	94142	4.53%	0.545%
17	7.686	1000	1003	1011	rBV	695328	686851	33.08%	3.978%
18	8.092	1066	1072	1079	rBV4	16681	37375	1.80%	0.216%
19	8.504	1136	1142	1147	rBV4	23083	35688	1.72%	0.207%
20	8.769	1182	1187	1190	rBV	2280133	2076521	100.00%	12.027%
21	9.169	1252	1255	1259	rBV	68818	61992	2.99%	0.359%
22	9.433	1296	1300	1314	rVB	684021	604671	29.12%	3.502%
23	10.222	1430	1434	1446	rBV	1176317	1133765	54.60%	6.567%
24	10.904	1547	1550	1559	rVB	559512	509720	24.55%	2.952%
25	11.145	1587	1591	1600	rBV	29790	52185	2.51%	0.302%
26	11.469	1642	1646	1653	rBV3	17463	28802	1.39%	0.167%
27	12.245	1773	1778	1782	rBV6	17959	28659	1.38%	0.166%
28	12.292	1782	1786	1791	rVV	73629	108330	5.22%	0.627%
29	12.333	1791	1793	1796	rVB	34492	29875	1.44%	0.173%
30	12.492	1815	1820	1823	rBV	1730412	1633125	78.65%	9.459%
31	13.033	1909	1912	1915	rBV	24529	25146	1.21%	0.146%
32	13.298	1953	1957	1961	rBV	36144	44638	2.15%	0.259%
33	13.433	1978	1980	1989	rVB7	17642	34727	1.67%	0.201%
34	13.533	1993	1997	2005	rVB	512395	490449	23.62%	2.841%

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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-BF072517.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.721	2027	2029	2032	rBV3	15965	22582	1.09%	0.131%
36	14.180	2104	2107	2112	rBV3	21256	28055	1.35%	0.162%
37	14.780	2206	2209	2214	rVB7	20976	28707	1.38%	0.166%
38	14.827	2214	2217	2218	rBV2	23718	25493	1.23%	0.148%
39	14.868	2220	2224	2229	rBV	318644	386864	18.63%	2.241%
40	16.009	2416	2418	2422	rBV5	20394	23258	1.12%	0.135%
41	16.104	2429	2434	2436	rBV5	26574	42850	2.06%	0.248%
42	16.321	2468	2471	2473	rBV3	20587	26615	1.28%	0.154%
43	16.456	2492	2494	2497	rBV4	22595	23642	1.14%	0.137%
44	16.562	2509	2512	2515	rBV5	19684	35937	1.73%	0.208%

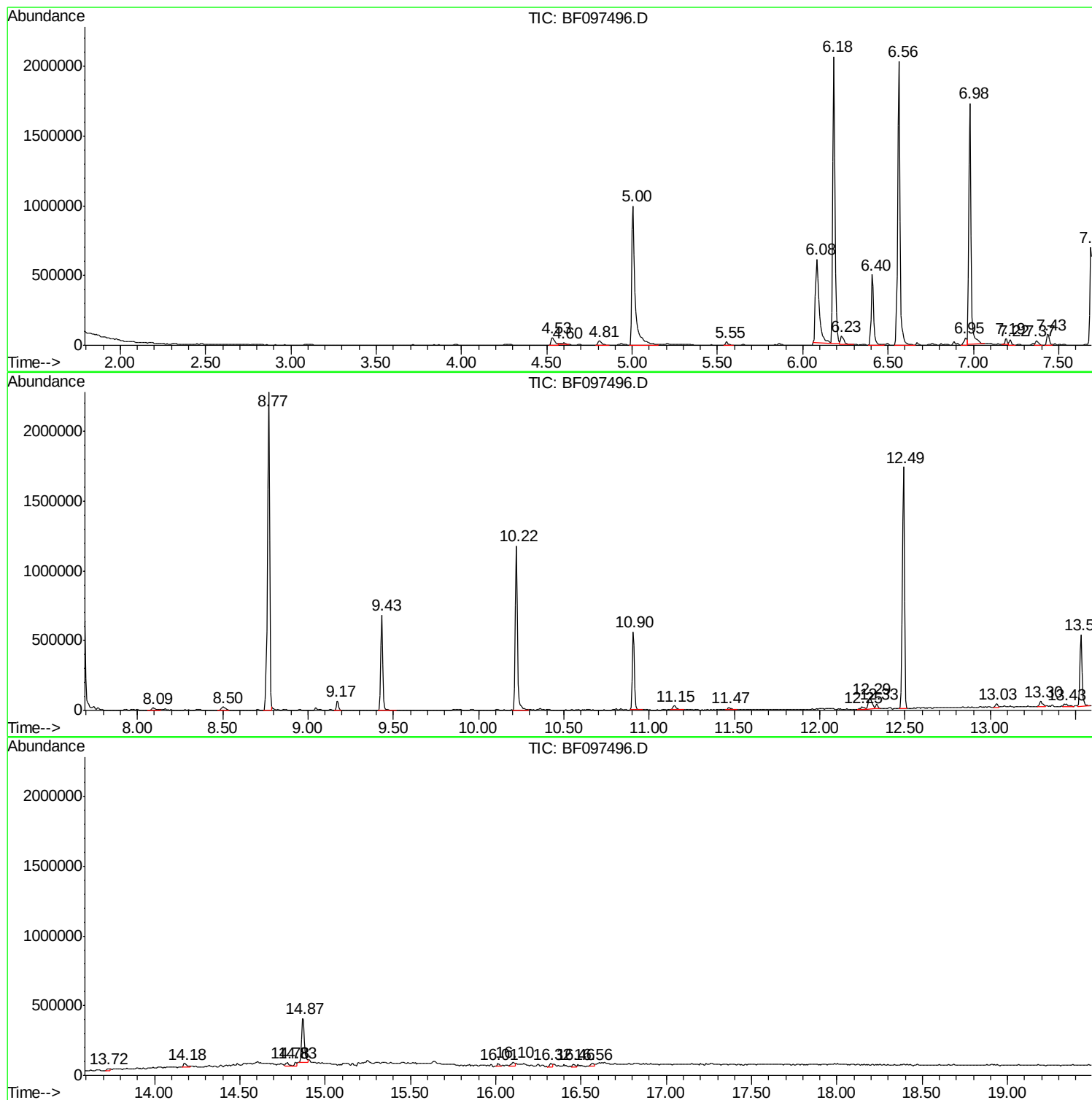
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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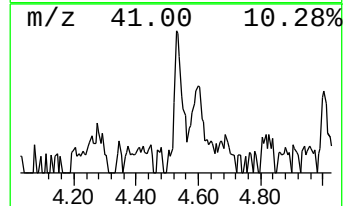
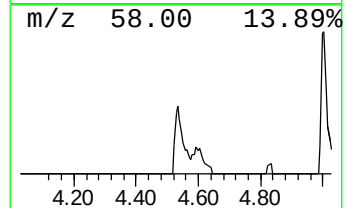
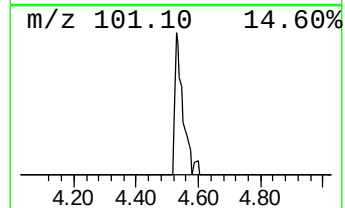
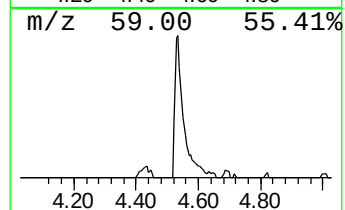
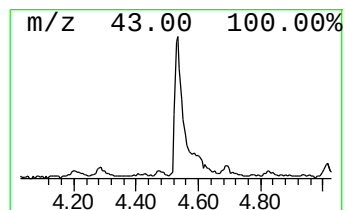
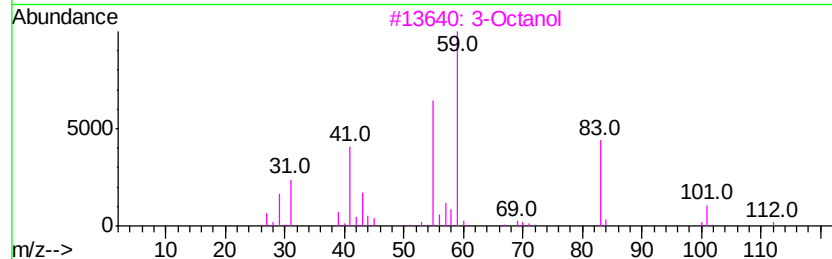
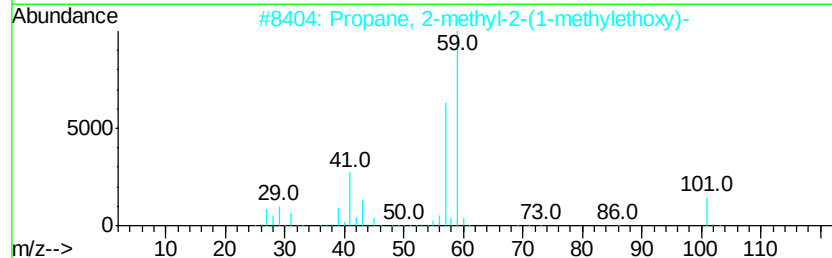
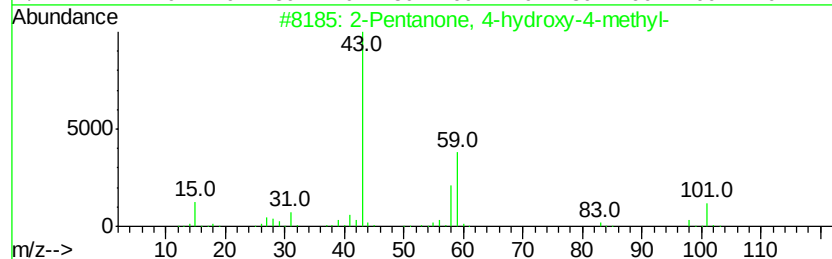
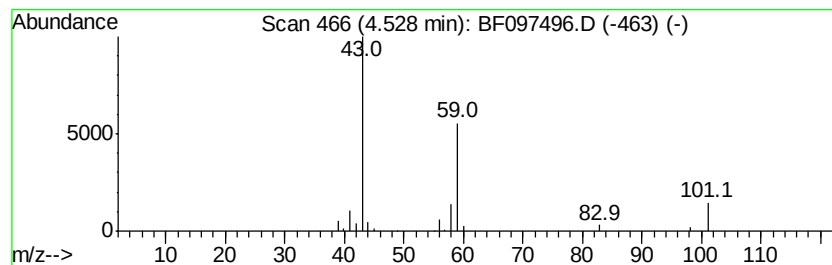
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.53	3.52 ng	88886	1,4-Dichlorobenzene-d4	6.40

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2		000123-42-2	56
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O		017348-59-3	36
3	3-Octanol	130	C8H18O		000589-98-0	33
4	2-Hexanol, 2-methyl-	116	C7H16O		000625-23-0	28
5	Ethanone, 1-(2-methylcyclopropyl)-	98	C6H10O		000930-56-3	9



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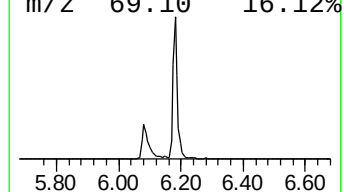
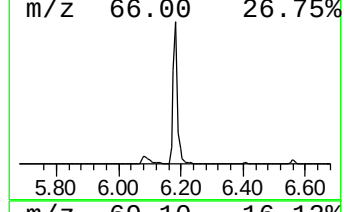
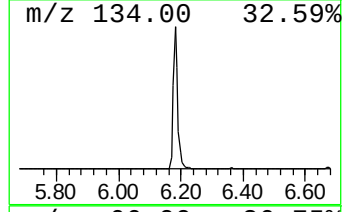
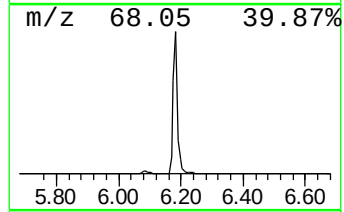
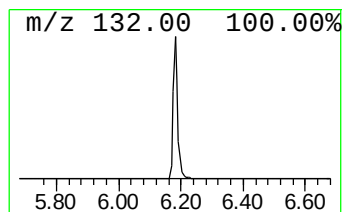
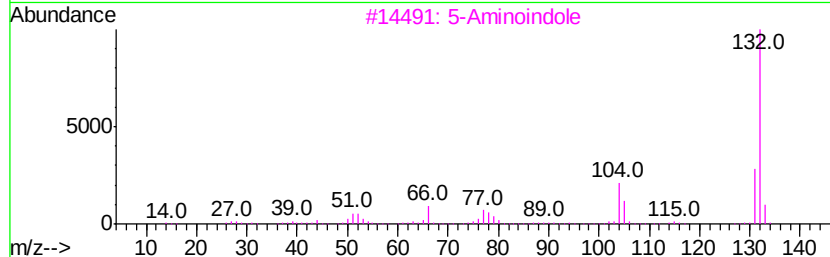
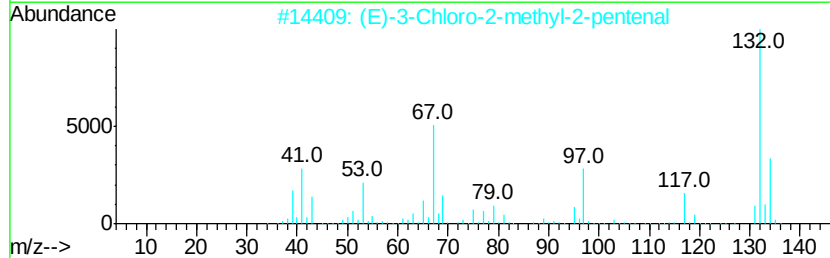
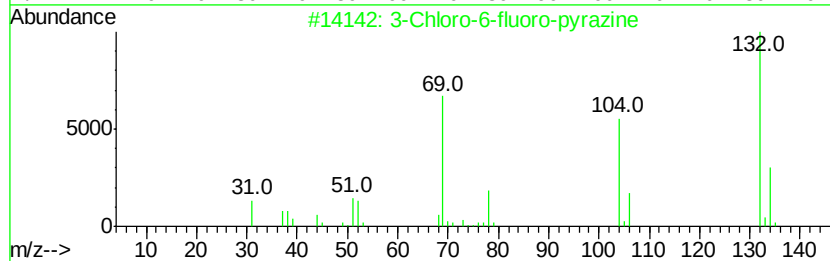
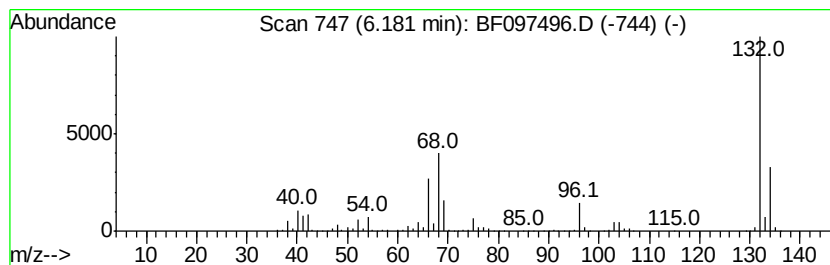
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.18 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.18	80.44 ng	2032100	1,4-Dichlorobenzene-d4	6.40

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		1-Aminoindan	133	C9H11N	034698-41-4	9



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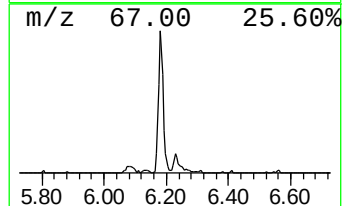
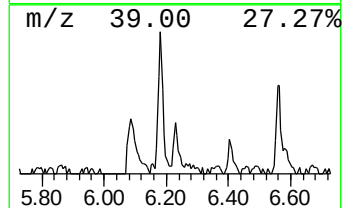
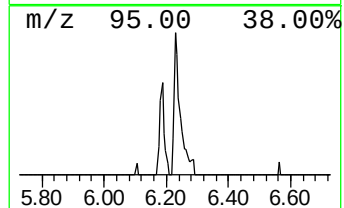
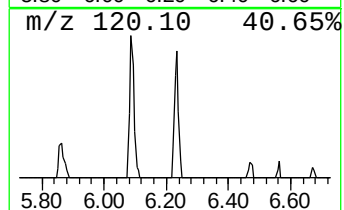
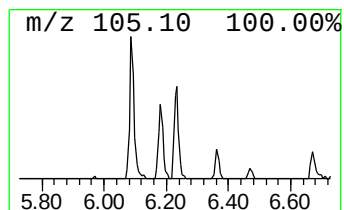
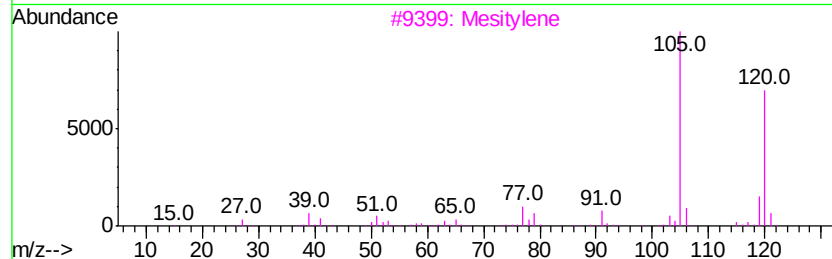
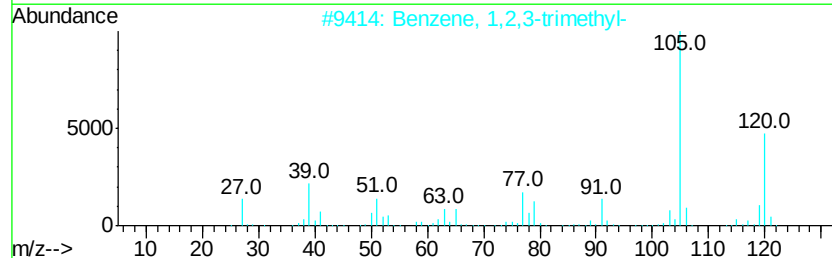
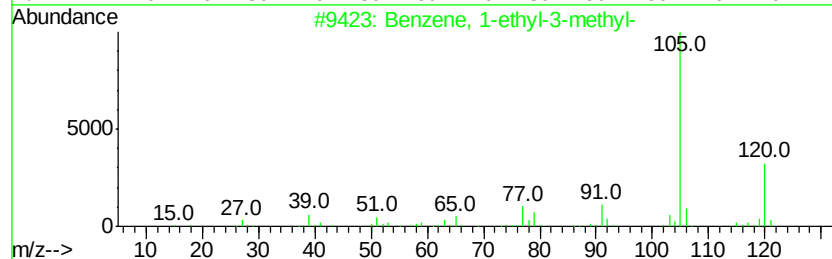
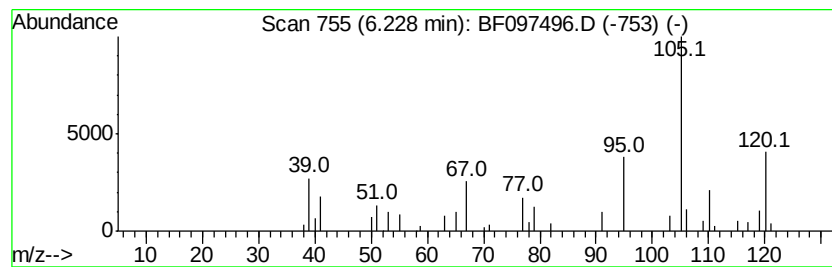
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzene, 1-ethyl-3-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.23	3.20 ng	80840	1,4-Dichlorobenzene-d4	6.40

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	55
2		Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	55
3		Mesitylene	120	C9H12	000108-67-8	55
4		Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	55
5		Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	50



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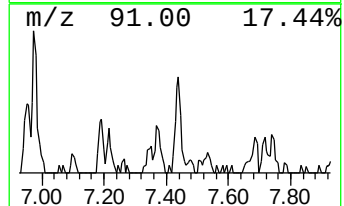
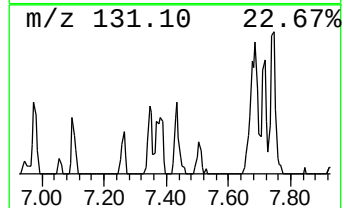
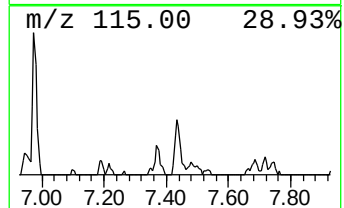
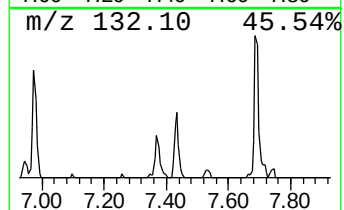
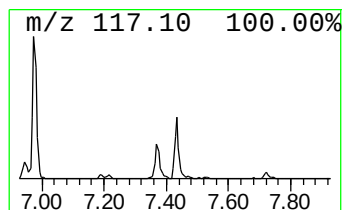
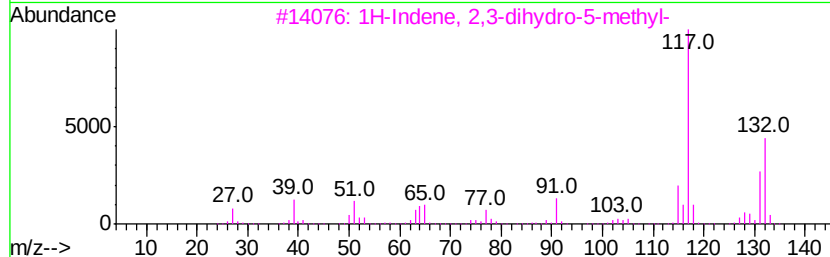
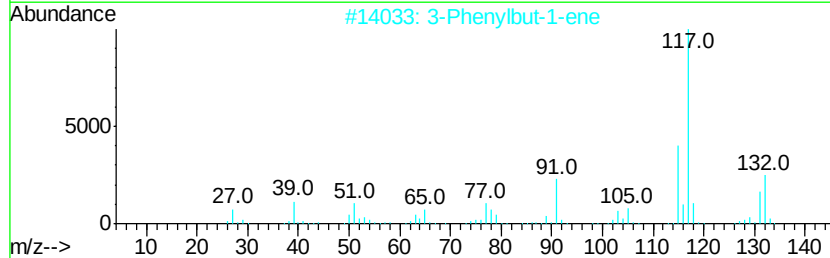
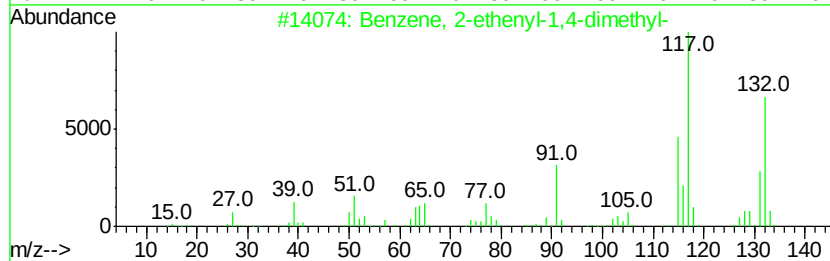
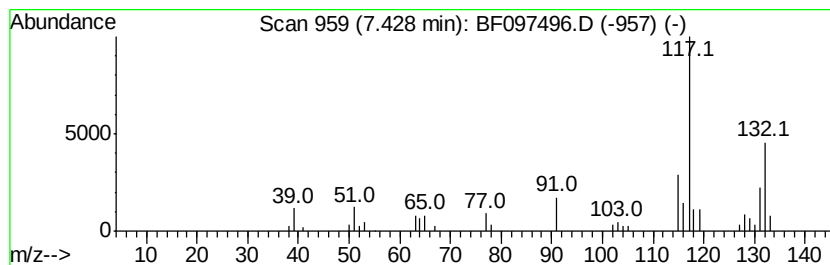
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.43	2.74 ng	94142	Napthalene-d8	7.69

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	96
2		3-Phenylbut-1-ene	132	C10H12	000934-10-1	87
3		1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	81
4		1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	81
5		1-Phenyl-1-butene	132	C10H12	000824-90-8	76



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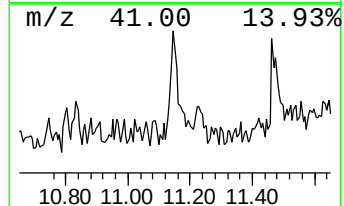
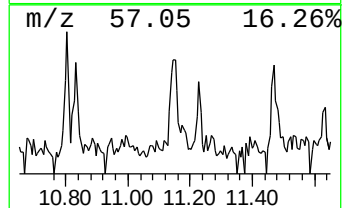
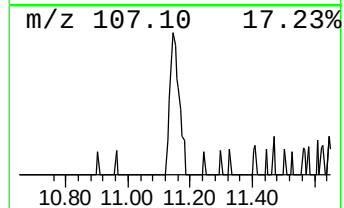
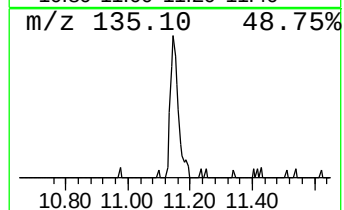
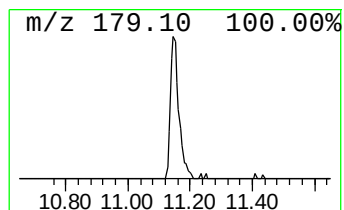
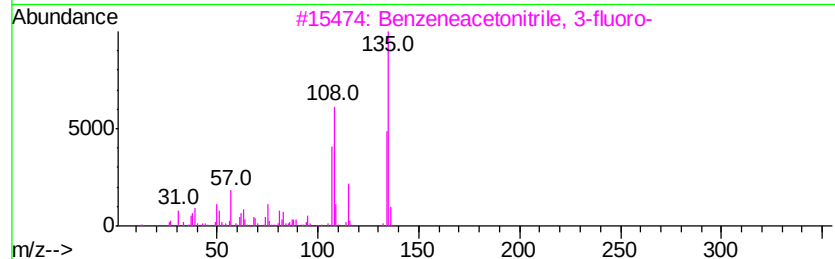
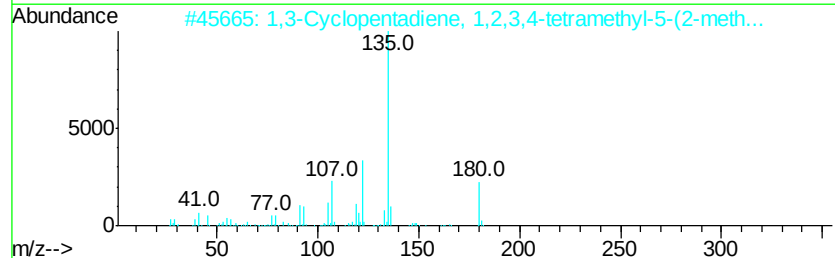
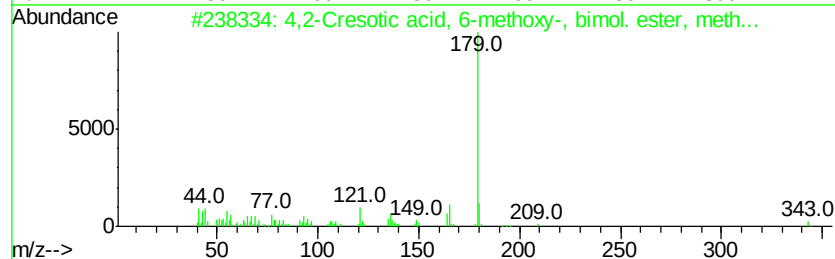
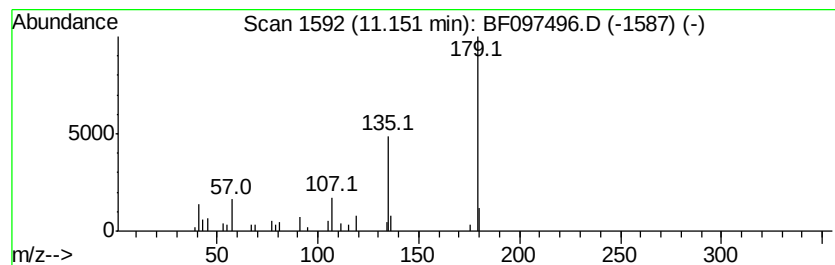
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 unknown11.15 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.15	2.05 ng	52185	Phenanthrene-d10	10.90

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,2-Cresotic acid, 6-methoxy-, b...	538	C29H30O10	019314-74-0	28		
2	1,3-Cyclopentadiene, 1,2,3,4-tet...	180	C12H20O	151226-45-8	27		
3	Benzeneacetonitrile, 3-fluoro-	135	C8H6FN	000501-00-8	12		
4	3,4-Methylenedioxyphenylacetic acid	180	C9H8O4	002861-28-1	10		
5	4-Methoxy-3-methylphenylacetic acid	180	C10H12O3	004513-73-9	10		



Data Path : Z:\HPCHEM1\BNA F\DATA\BF080817\
Data File : BF097496.D
Acq On : 9 Aug 2017 4:10
Operator : SJ/JU
Sample : I4604-02
Misc :
ALS Vial : 22 Sample Multiplier: 1

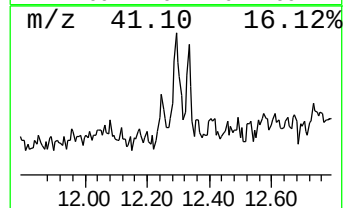
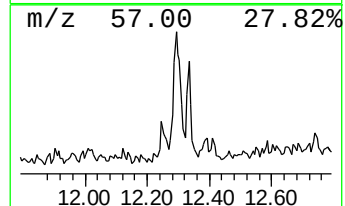
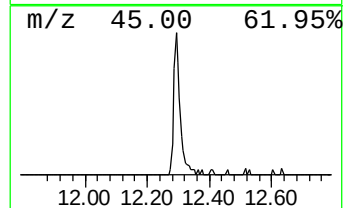
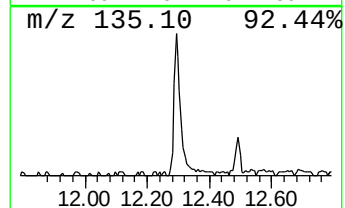
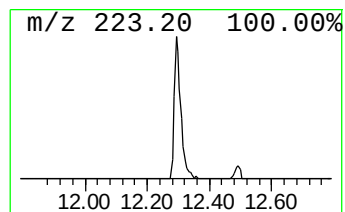
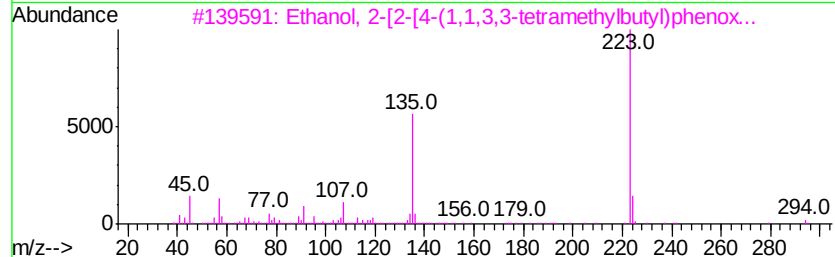
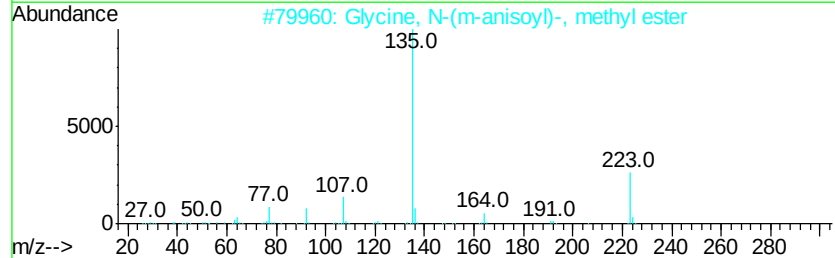
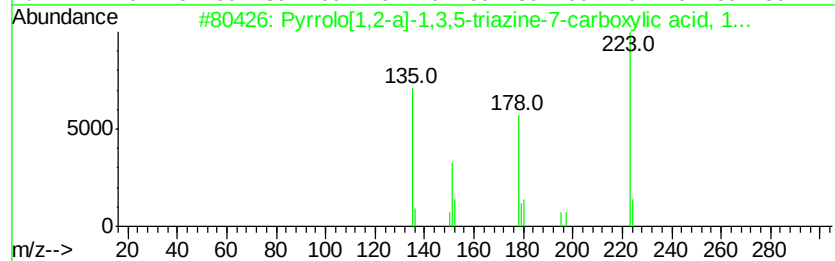
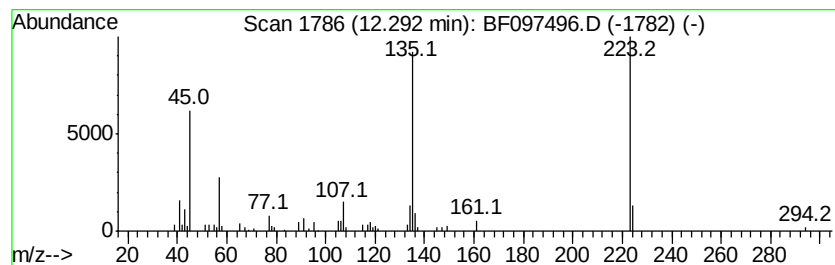
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ClientSampleId :
MW-2A-080217

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Pyrrolo[1,2-a]-1,3,5-triazi... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.29	4.42 ng	108330	Chrysene-d12	13.53	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrrolo[1,2-a]-1,3,5-triazine-7-...	223	C9H9N3O4	054449-89-7	90
2	Glycine, N-(m-anisoyl)-, methyl ...	223	C11H13N04	1000299-70-7	59
3	Ethanol, 2-[2-[4-(1,1,3,3-tetram...	294	C18H30O3	002315-61-9	49
4	Hexestrol	270	C18H22O2	000084-16-2	43
5	((1,2-Diethylethylene)bis(p-phen...	354	C22H26O4	004547-76-6	35



Data Path : Z:\HPCHEM1\BNA F\DATA\BF080817\
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Sample : I4604-02
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-2A-080217

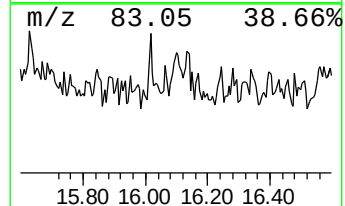
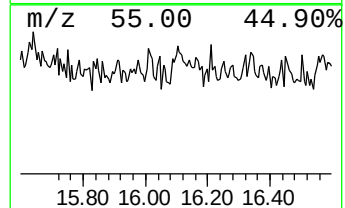
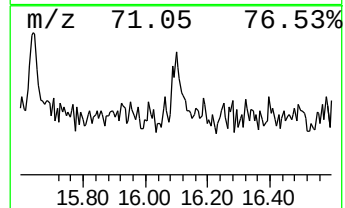
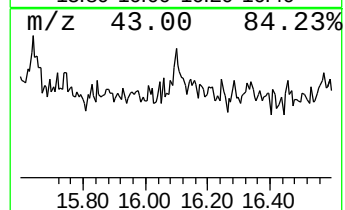
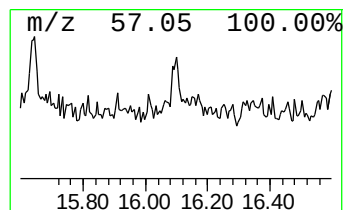
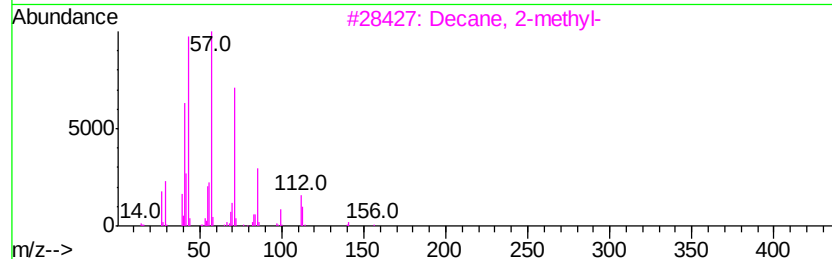
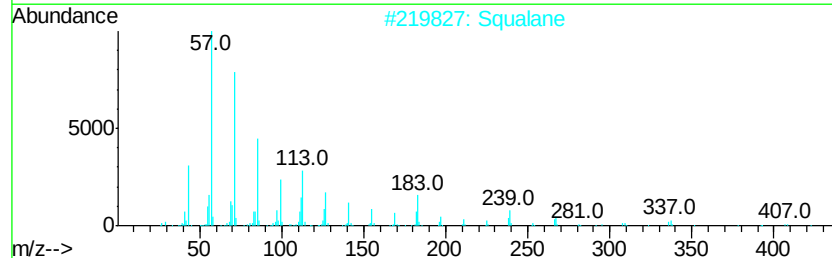
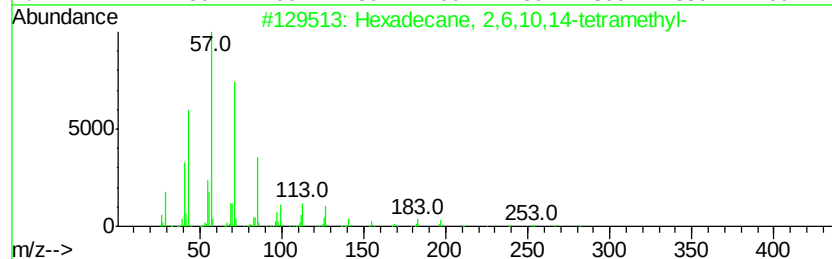
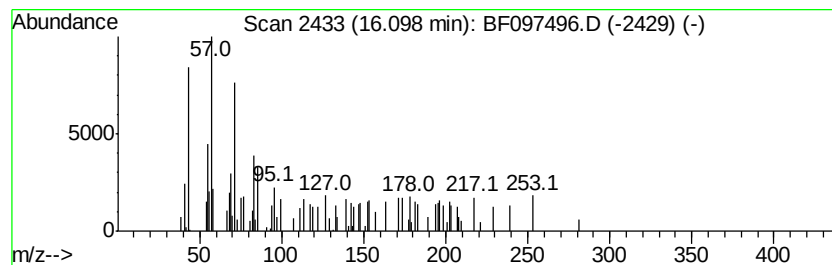
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown16.10 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.10	2.22 ng	42850	Perylene-d12	14.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	38
2		Squalane	422	C30H62	000111-01-3	38
3		Decane, 2-methyl-	156	C11H24	006975-98-0	35
4		Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	35
5		Tridecane, 6-methyl-	198	C14H30	013287-21-3	35



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Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-2A-080217

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.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
2-Pentanone, 4-hy...	4.53	3.5	ng	88886	1	6.40	505258	20.0
unknown6.18	6.18	80.4	ng	2032100	1	6.40	505258	20.0
Benzene, 1-ethyl-...	6.23	3.2	ng	80840	1	6.40	505258	20.0
Benzene, 2-etheny...	7.43	2.7	ng	94142	2	7.69	686851	20.0
unknown11.15	11.15	2.0	ng	52185	4	10.90	509720	20.0
Pyrrolo[1,2-a]-1,...	12.29	4.4	ng	108330	5	13.53	490449	20.0
unknown16.10	16.10	2.2	ng	42850	6	14.87	386864	20.0