

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF092418\
 Data File : BF109266.D
 Acq On : 24 Sep 2018 14:42
 Operator : JU/SJ
 Sample : J5044-09
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 GRID09-COMP-092018

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-BF092218.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	4.899	474	478	487	rBV	62951	76830	3.57%	0.384%
2	5.316	544	549	552	rBV	1953830	1780738	82.74%	8.899%
3	6.346	719	724	735	rBV	2053183	1964130	91.26%	9.816%
4	6.475	742	746	749	rBV	2269811	1907809	88.64%	9.534%
5	6.704	782	785	789	rBV	757643	635414	29.52%	3.175%
6	6.863	808	812	815	rBV	1916848	1504678	69.91%	7.520%
7	7.263	876	880	883	rBV	1279902	1201597	55.83%	6.005%
8	7.987	999	1003	1006	rBV	1038633	822274	38.20%	4.109%
9	9.063	1182	1186	1189	rBV	2625261	2152317	100.00%	10.756%
10	9.457	1249	1253	1256	rBV	489815	386674	17.97%	1.932%
11	9.734	1297	1300	1304	rVB2	1032111	903721	41.99%	4.516%
12	10.522	1430	1434	1437	rBV	1301372	1222544	56.80%	6.110%
13	11.210	1548	1551	1554	rBV	933225	842857	39.16%	4.212%
14	11.233	1554	1555	1558	rVV	157345	92179	4.28%	0.461%
15	11.286	1558	1564	1567	rVB	60820	52446	2.44%	0.262%
16	11.751	1639	1643	1646	rBV2	61687	68447	3.18%	0.342%
17	11.822	1652	1655	1658	rBV2	24617	27383	1.27%	0.137%
18	12.416	1753	1756	1760	rBV	123451	102264	4.75%	0.511%
19	12.645	1789	1795	1798	rBV2	96101	105261	4.89%	0.526%
20	12.792	1816	1820	1824	rVB	1905220	1566107	72.76%	7.827%
21	13.039	1856	1862	1865	rBV	27353	28101	1.31%	0.140%
22	13.280	1897	1903	1910	rBV	127179	133268	6.19%	0.666%
23	13.704	1972	1975	1982	rBV2	65409	102068	4.74%	0.510%
24	13.839	1992	1998	2000	rBV	853965	832846	38.70%	4.162%
25	13.863	2000	2002	2004	rVB	49875	37736	1.75%	0.189%
26	14.327	2078	2081	2086	rVB5	30066	43738	2.03%	0.219%
27	14.474	2103	2106	2110	rBV	60583	69388	3.22%	0.347%
28	14.621	2128	2131	2136	rBV	41475	40744	1.89%	0.204%
29	14.692	2139	2143	2146	rVB	185913	188909	8.78%	0.944%
30	14.845	2165	2169	2170	rBV	40267	49092	2.28%	0.245%
31	14.933	2181	2184	2188	rVB2	48161	54936	2.55%	0.275%
32	15.174	2222	2225	2231	rVB	43498	59184	2.75%	0.296%
33	15.239	2231	2236	2240	rBV	645277	765499	35.57%	3.826%
34	15.286	2241	2244	2248	rVB2	48996	59458	2.76%	0.297%

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ALS Vial : 13 Sample Multiplier: 1

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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

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35	15.686	2309	2312	2317	rVB2	53653	77875	3.62%	0.389%
36	16.151	2388	2391	2396	rVB	36365	51399	2.39%	0.257%

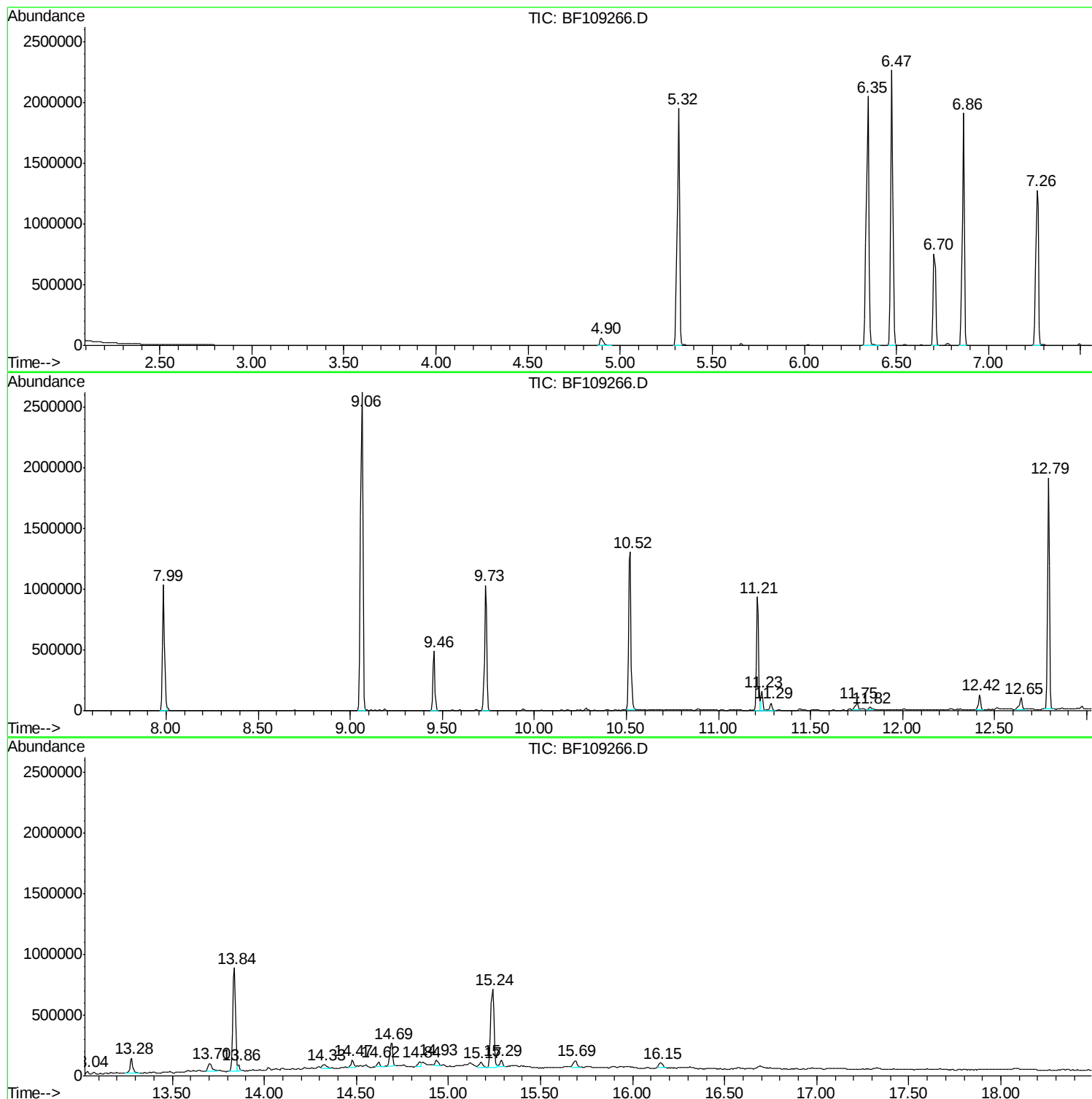
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF092218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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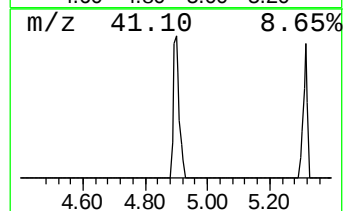
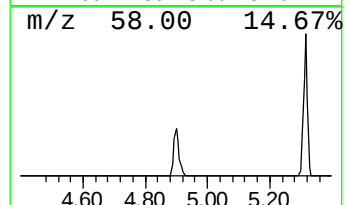
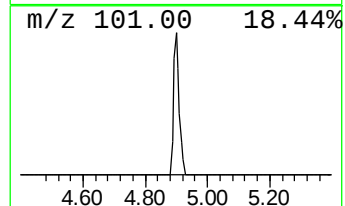
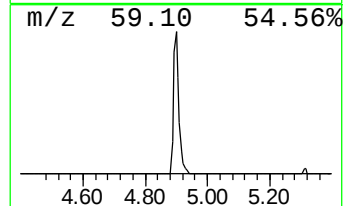
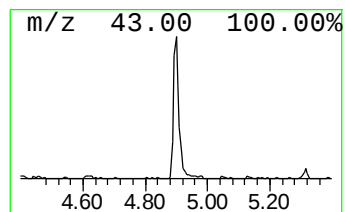
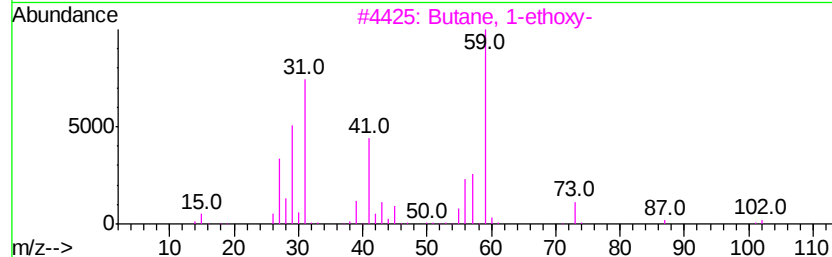
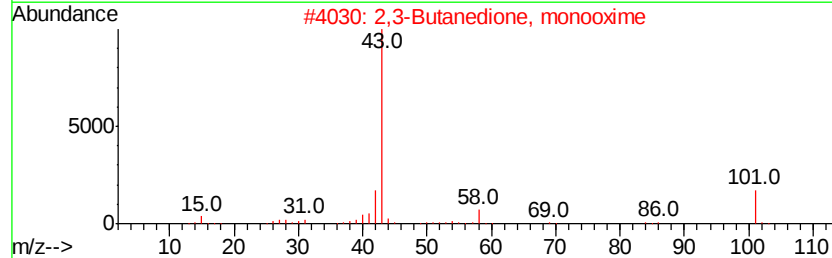
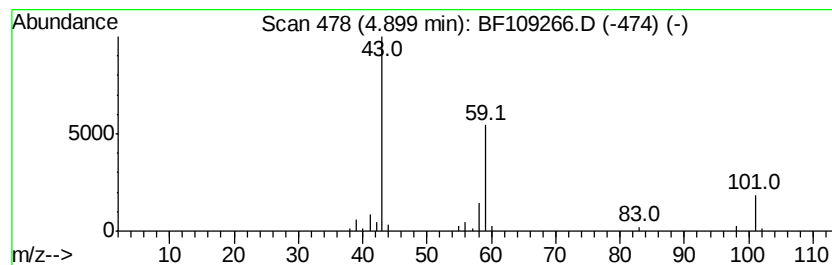
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.90	2.42 ng	76830	1,4-Dichlorobenzene-d4	6.70

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
3			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			Cycloserine	102	C3H6N2O2	000068-41-7	9



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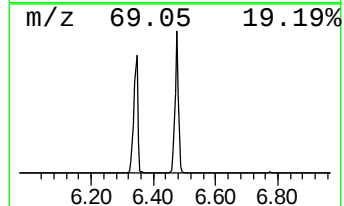
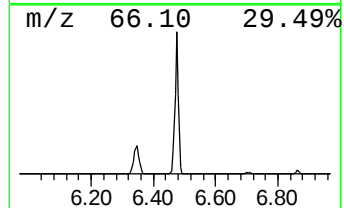
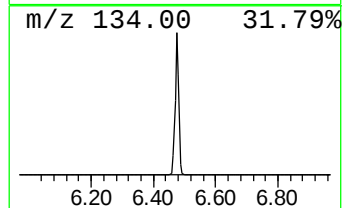
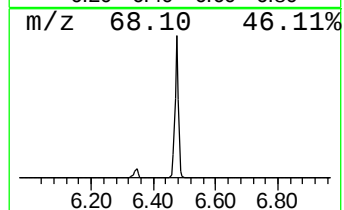
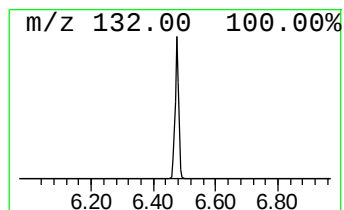
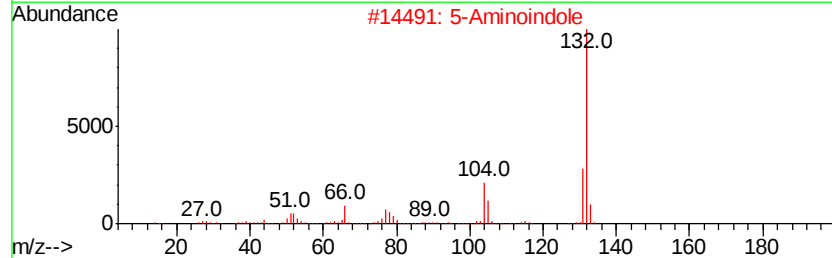
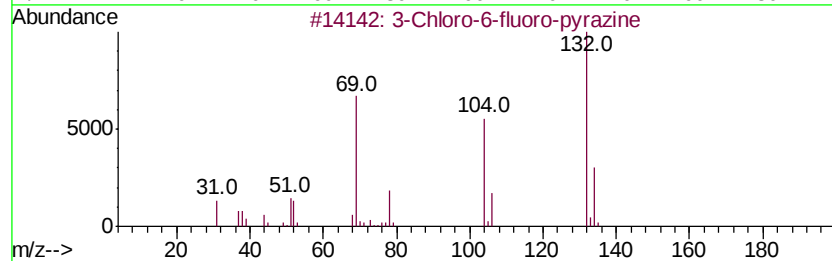
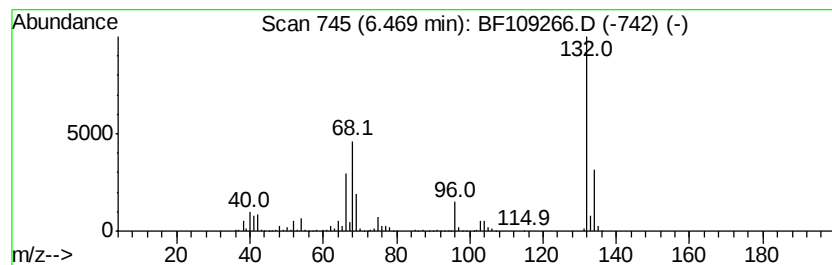
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.47 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.47	60.05 ng	1907810	1,4-Dichlorobenzene-d4	6.70

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2			5-Aminoindole	132	C8H8N2	005192-03-0	12
3			Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	10
4			Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5			Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9



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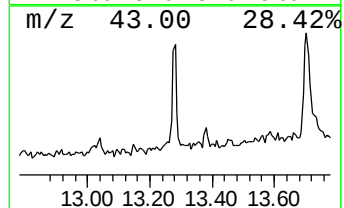
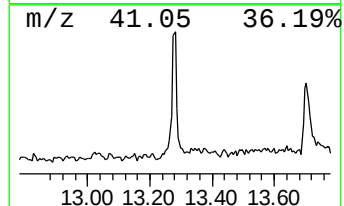
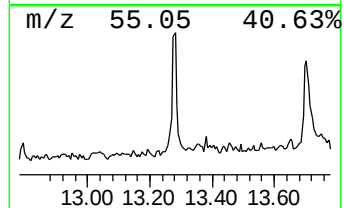
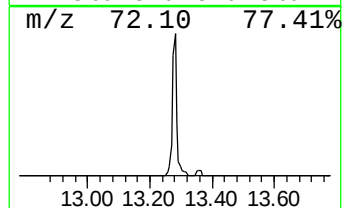
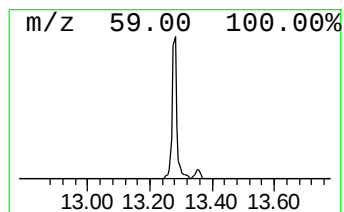
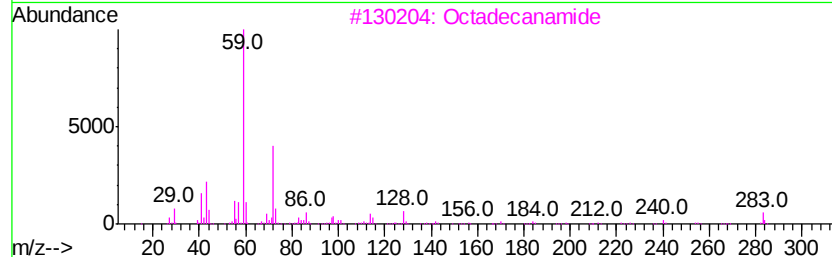
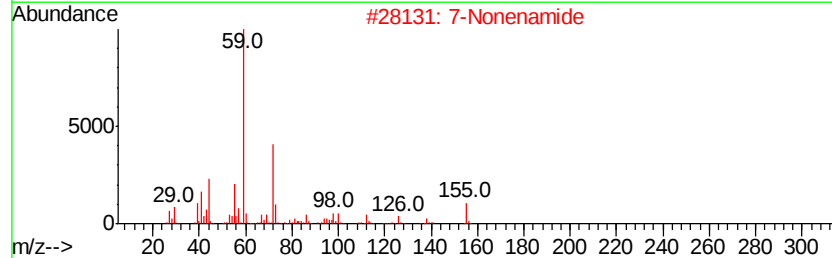
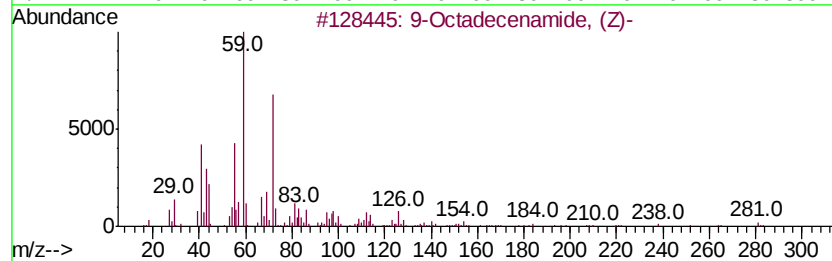
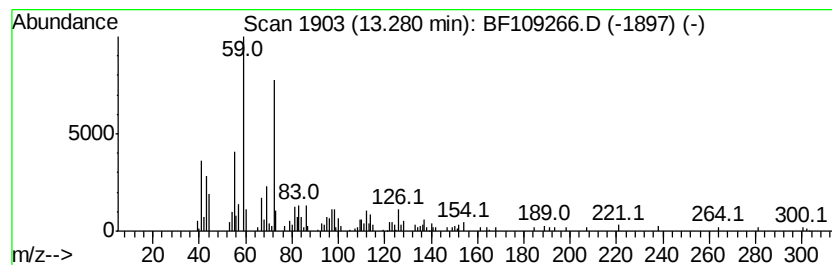
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.28	3.20 ng	133268	Chrysene-d12	13.84

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	99
2		7-Nonenamide	155	C9H17NO	090949-53-4	53
3		Octadecanamide	283	C18H37NO	000124-26-5	50
4		Octanamide	143	C8H17NO	000629-01-6	43
5		Dodecanamide	199	C12H25NO	001120-16-7	43



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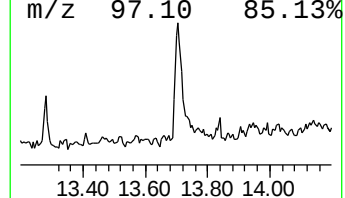
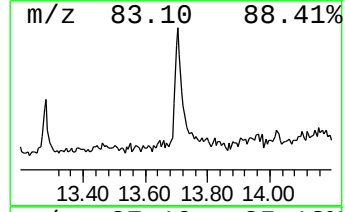
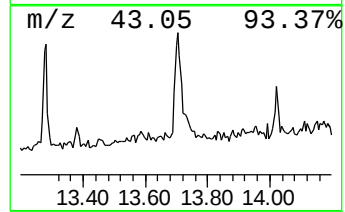
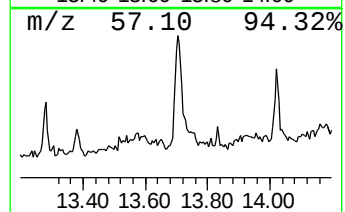
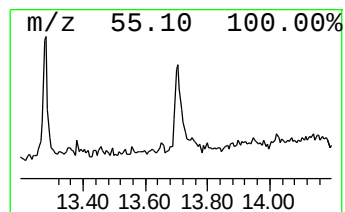
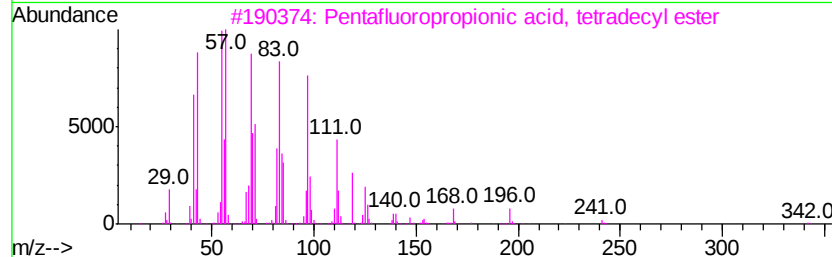
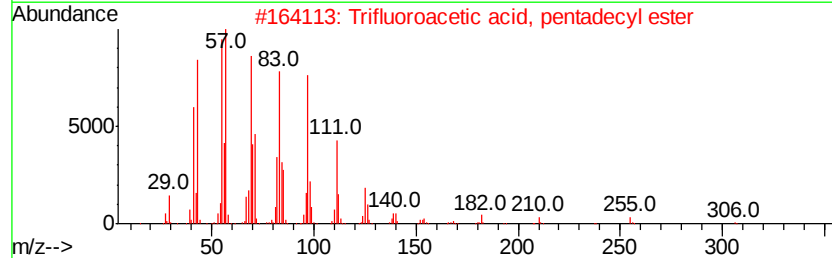
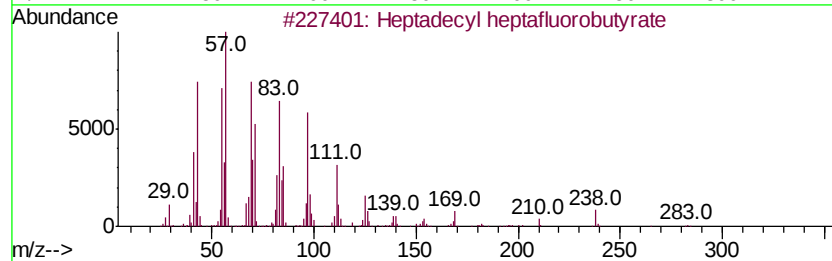
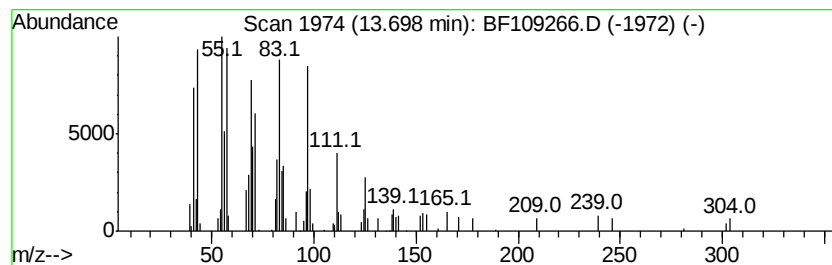
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Heptadecyl heptafluorobutyrate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.70	2.45 ng	102068	Chrysene-d12	13.84

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	90
2			Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	87
3			Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	87
4			Trifluoroacetoxv hexadecane	338	C18H33F3O2	006222-03-3	87
5			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	87



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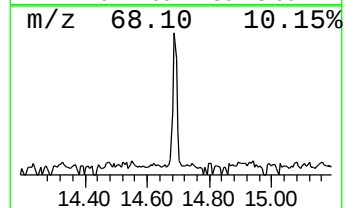
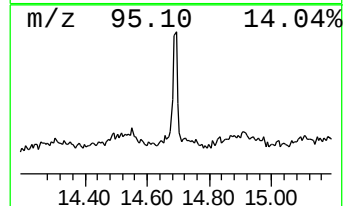
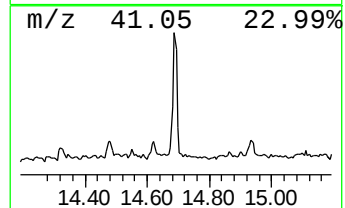
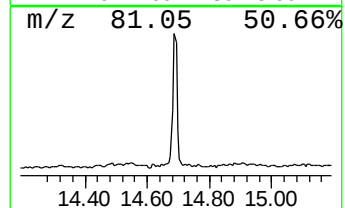
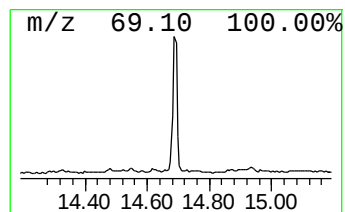
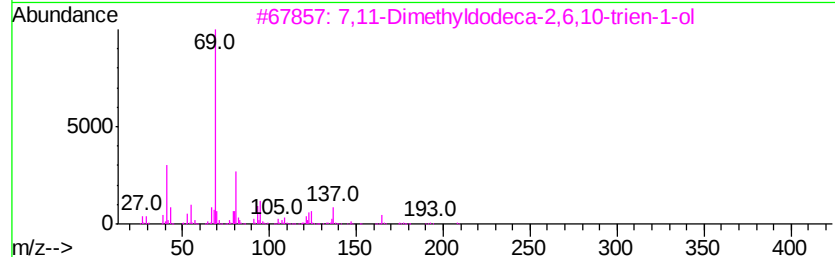
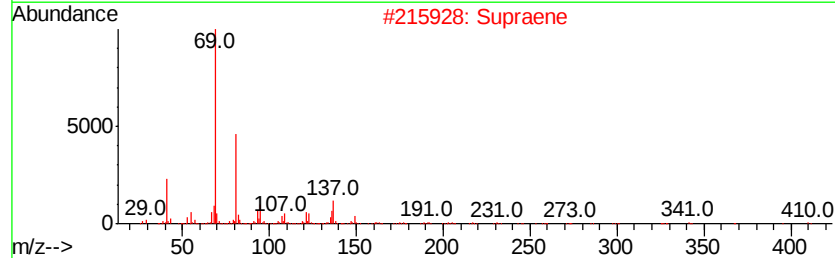
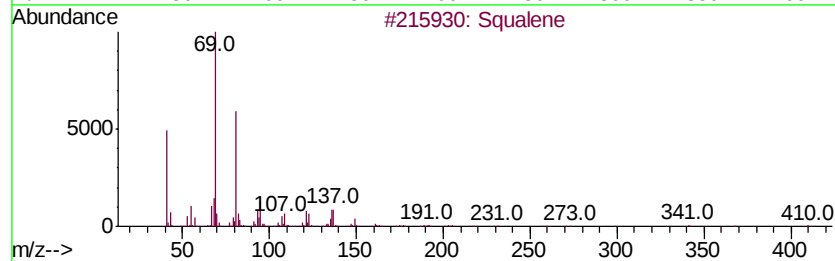
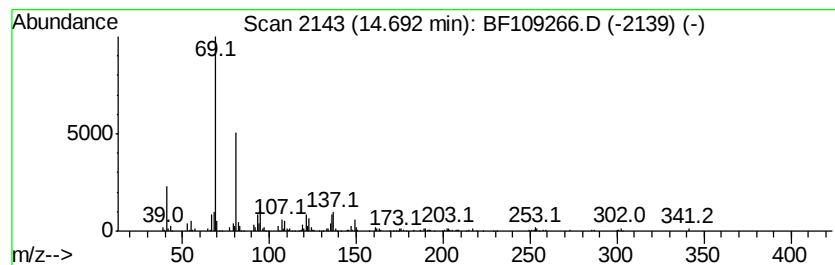
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Peak Number 7 Squalene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.69	4.94 ng	188909	Perylene-d12	15.24

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	91
2		Supraene	410	C30H50	007683-64-9	91
3		7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	83
4		trans-Farnesol	222	C15H26O	000106-28-5	64
5		2,6,10-Dodecatrien-1-ol, 3,7,11-...	264	C17H28O2	004128-17-0	59



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Misc :
ALS Vial : 13 Sample Multiplier: 1

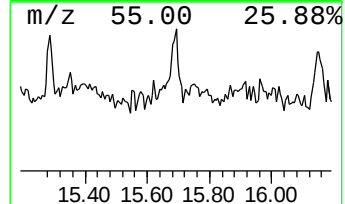
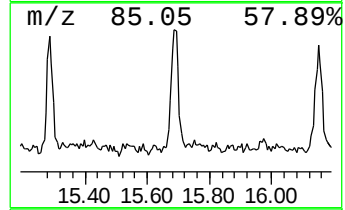
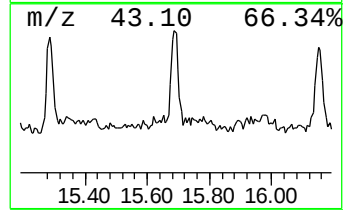
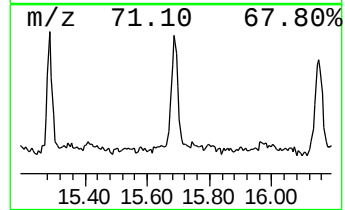
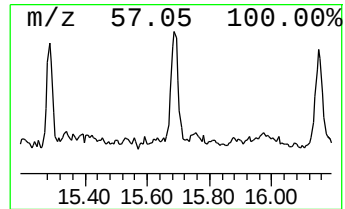
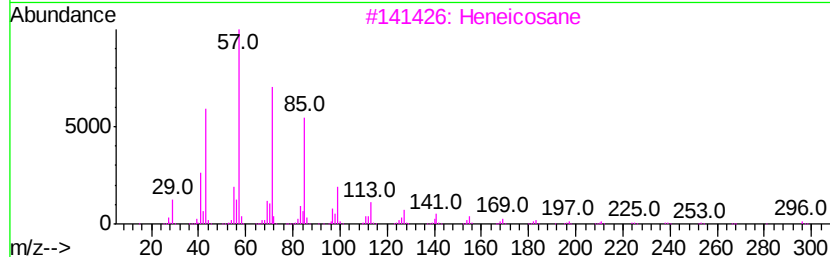
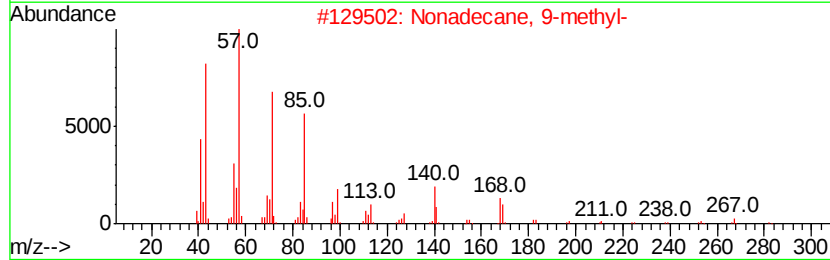
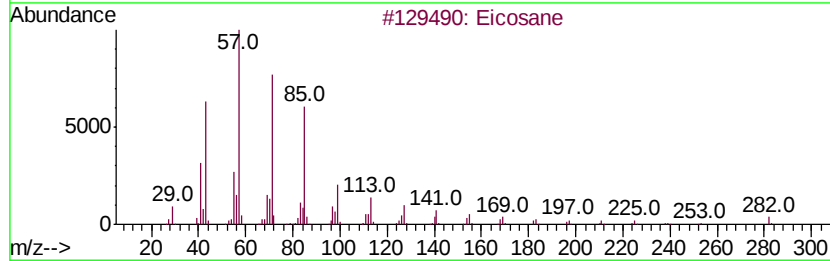
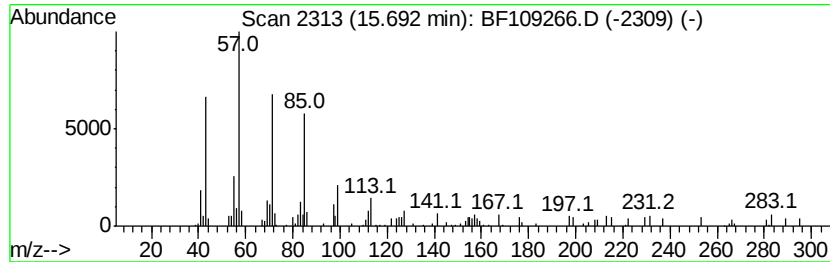
Instrument :
BNA_F
ClientSampleId :
GRID09-COMP-092018

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF092218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.69	2.03 ng	77875	Perylene-d12	15.24
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Eicosane	282 C20H42	000112-95-8	95
2	Nonadecane, 9-methyl-	282 C20H42	013287-24-6	94
3	Heneicosane	296 C21H44	000629-94-7	87
4	10-Methylnonadecane	282 C20H42	056862-62-5	86
5	Heptadecane	240 C17H36	000629-78-7	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF092418\
Data File : BF109266.D
Acq On : 24 Sep 2018 14:42
Operator : JU/SJ
Sample : J5044-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GRID09-COMP-092018

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.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...	4.90	2.4	ng	76830	1	6.70	635414	20.0
unknown6.47	6.47	60.0	ng	1907810	1	6.70	635414	20.0
9-Octadecenamide, ...	13.28	3.2	ng	133268	5	13.84	832846	20.0
Heptadecyl heptaf...	13.70	2.5	ng	102068	5	13.84	832846	20.0
Squalene	14.69	4.9	ng	188909	6	15.24	765499	20.0
Eicosane	15.69	2.0	ng	77875	6	15.24	765499	20.0