

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF091318\
 Data File : BF108977.D
 Acq On : 13 Sep 2018 21:04
 Operator : JU/SJ
 Sample : J4875-05
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 091118-DBRI-F-D-B

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-BF090518.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	4.907	434	437	445	rBV	139164	157474	3.47%	0.521%
2	5.331	505	509	513	rBV	1488016	1390692	30.62%	4.604%
3	6.354	679	683	692	rBV	1289995	1011660	22.27%	3.350%
4	6.495	700	707	710	rBV	2876229	2476070	54.51%	8.198%
5	6.725	743	746	750	rBV	942593	849842	18.71%	2.814%
6	6.889	769	774	777	rBV	3308034	3124898	68.80%	10.346%
7	7.289	837	842	845	rBV	2757371	2720352	59.89%	9.007%
8	8.007	960	964	968	rBV	1253211	1039739	22.89%	3.442%
9	9.089	1143	1148	1151	rBV	4880193	4542241	100.00%	15.039%
10	9.477	1210	1214	1217	rBV	498766	376553	8.29%	1.247%
11	9.760	1258	1262	1266	rBV	1364148	1156571	25.46%	3.829%
12	10.177	1329	1333	1336	rBV	89692	71601	1.58%	0.237%
13	10.436	1374	1377	1381	rVB	82404	67995	1.50%	0.225%
14	10.542	1391	1395	1398	rBV	2143487	1898869	41.80%	6.287%
15	11.236	1509	1513	1516	rBV	1313382	1059621	23.33%	3.508%
16	11.777	1601	1605	1614	rBV2	112714	133490	2.94%	0.442%
17	12.824	1778	1783	1786	rBV	4095133	4031618	88.76%	13.348%
18	13.065	1820	1824	1828	rBV	61072	51200	1.13%	0.170%
19	13.407	1879	1882	1884	rBV	91048	73372	1.62%	0.243%
20	13.736	1934	1938	1941	rBV	120063	121802	2.68%	0.403%
21	13.860	1955	1959	1963	rBV	1142314	973566	21.43%	3.223%
22	14.048	1983	1991	1995	rBV	149011	143729	3.16%	0.476%
23	14.354	2040	2043	2046	rBV	184070	148529	3.27%	0.492%
24	14.648	2089	2093	2098	rBV	198630	187024	4.12%	0.619%
25	14.718	2101	2105	2110	rVB	491469	449389	9.89%	1.488%
26	14.965	2143	2147	2154	rBV	181733	202393	4.46%	0.670%
27	15.265	2193	2198	2203	rBV	855387	1034684	22.78%	3.426%
28	15.324	2203	2208	2215	rVB	163417	205652	4.53%	0.681%
29	15.730	2272	2277	2286	rBV	141909	202811	4.46%	0.671%
30	16.201	2351	2357	2363	rVB	98350	158473	3.49%	0.525%
31	16.748	2444	2450	2457	rBV2	43007	85859	1.89%	0.284%
32	17.395	2555	2560	2571	rVB5	24358	55286	1.22%	0.183%

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Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
091118-DBRI-F-D-B

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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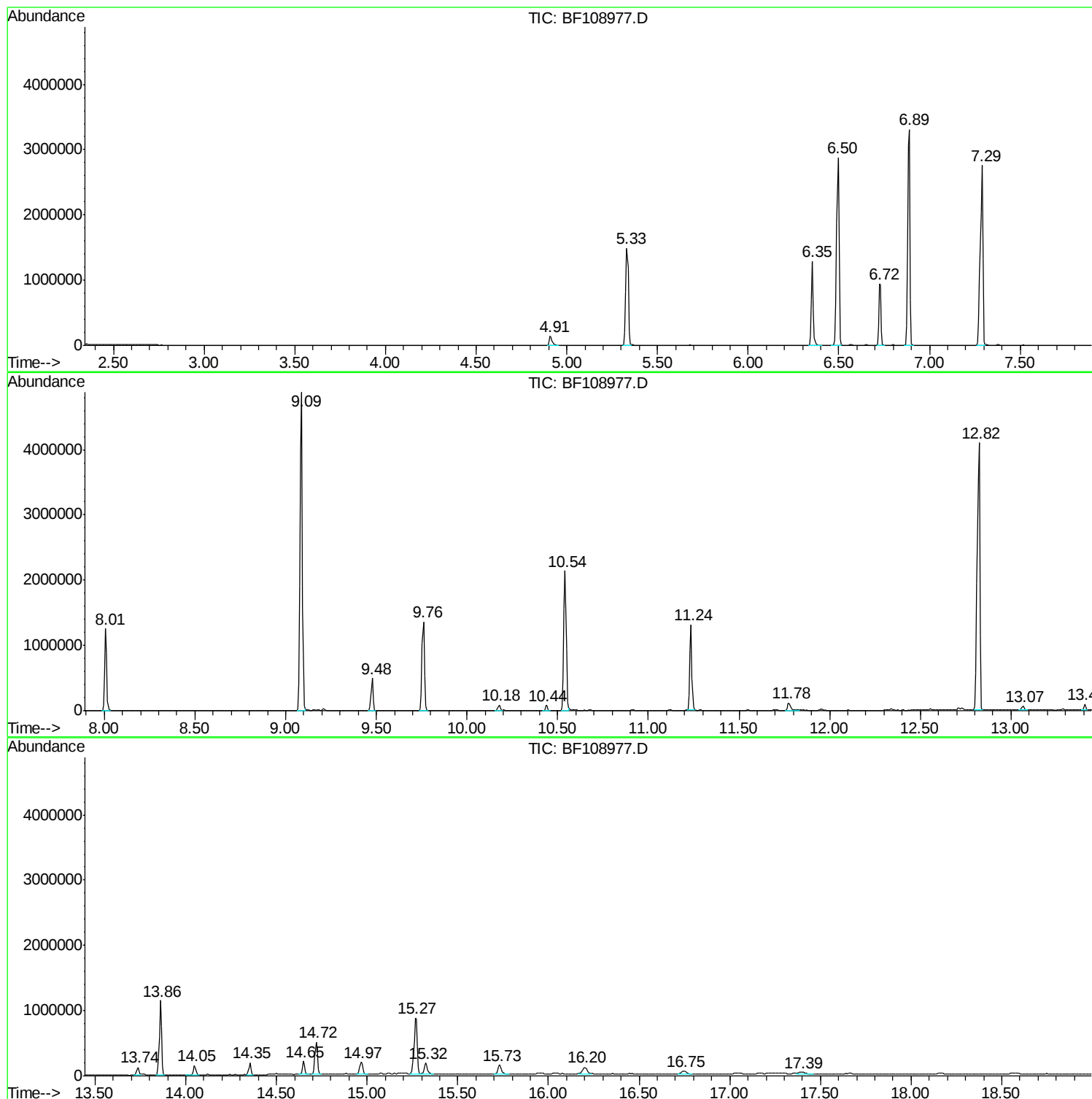
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF090518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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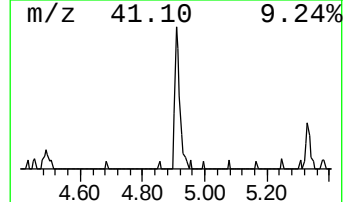
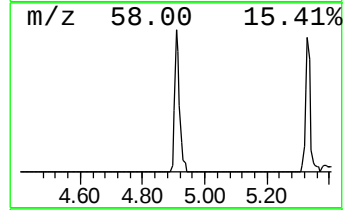
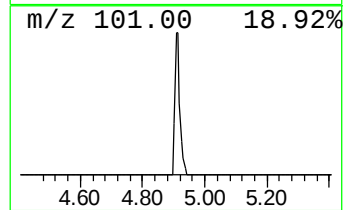
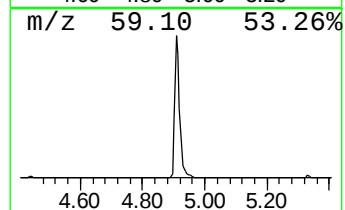
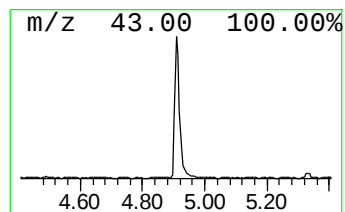
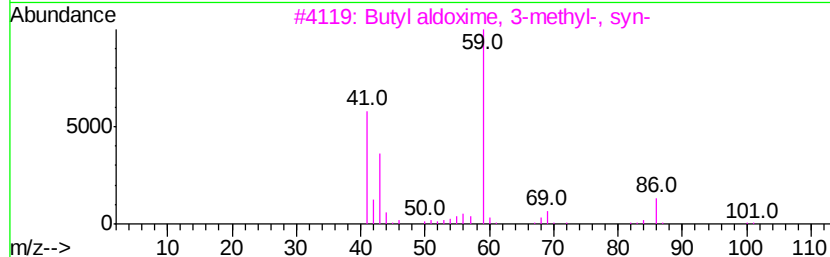
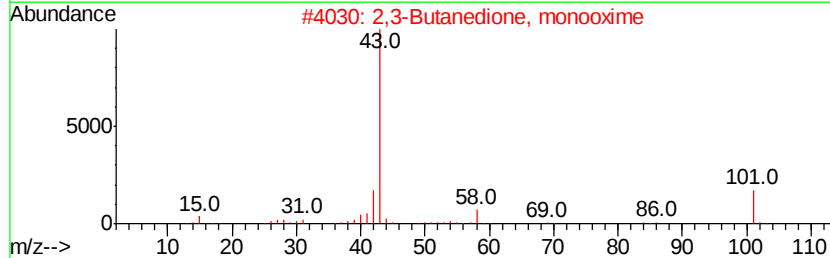
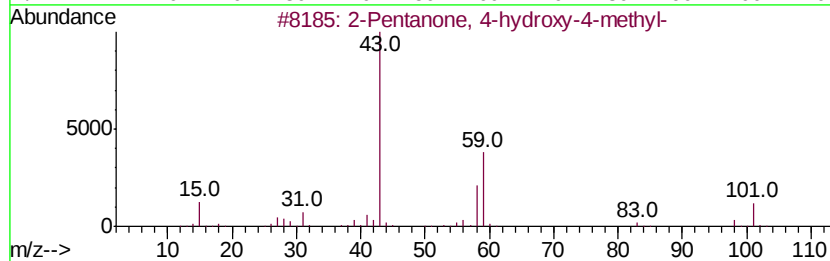
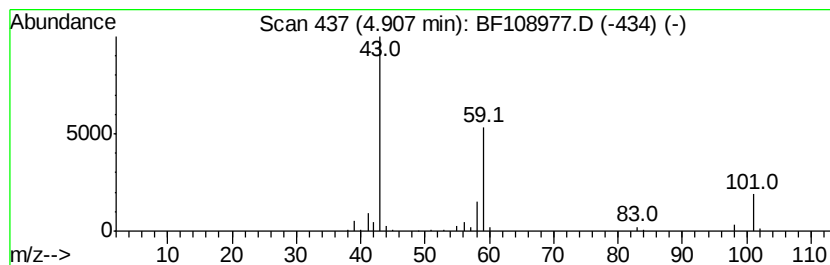
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.91	3.71 ng	157474	1,4-Dichlorobenzene-d4	6.73

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
3		Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	23
4		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5		Acetamide, N-(aminocarbonyl)-	102	C3H6N2O2	000591-07-1	9



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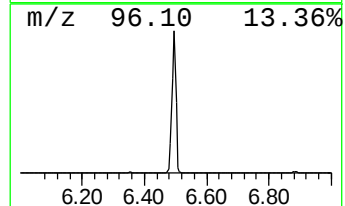
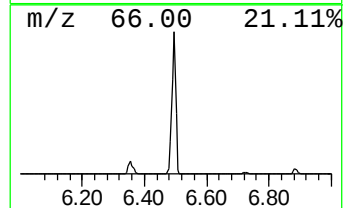
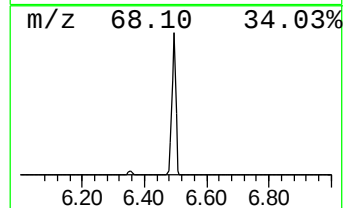
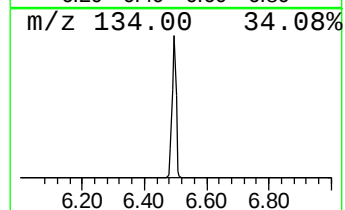
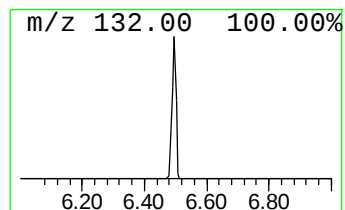
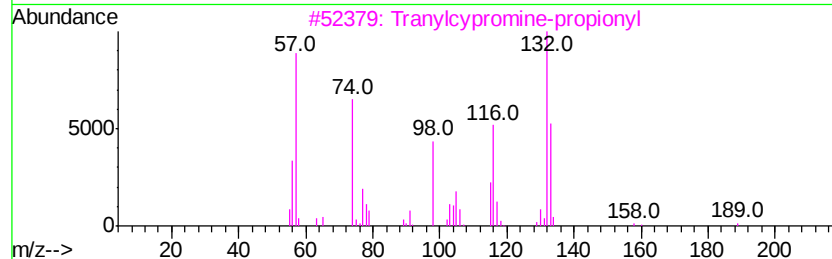
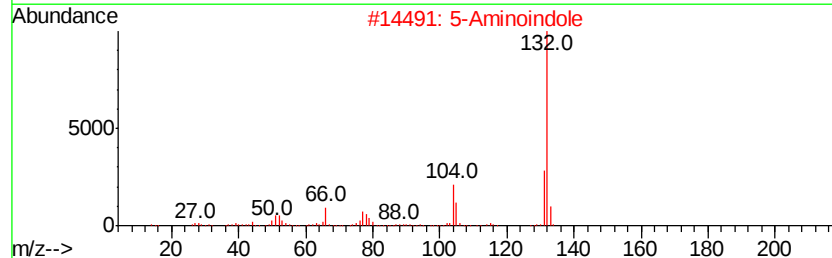
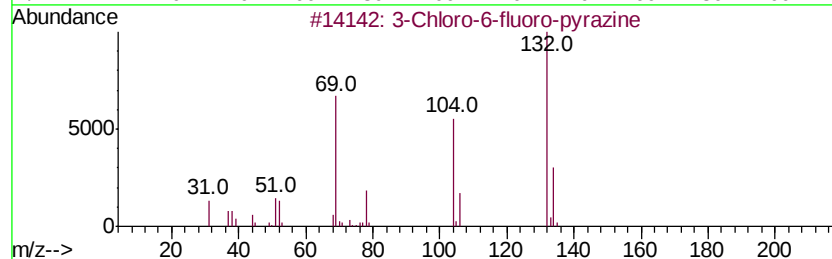
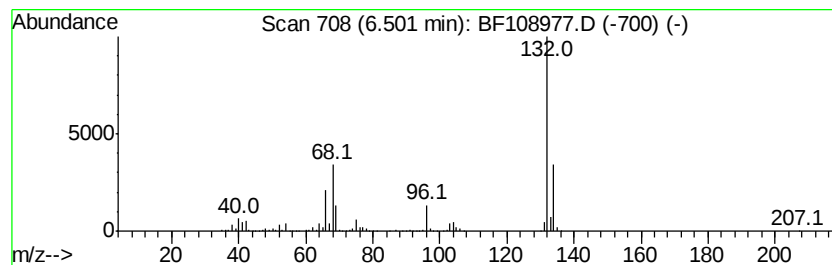
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.50 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	58.27 ng	2476070	1,4-Dichlorobenzene-d4	6.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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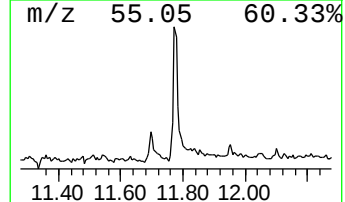
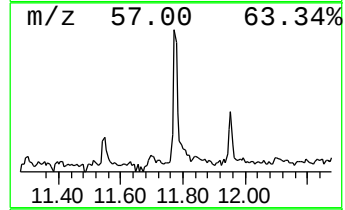
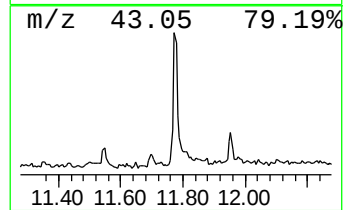
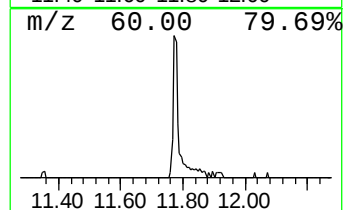
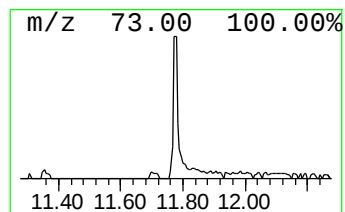
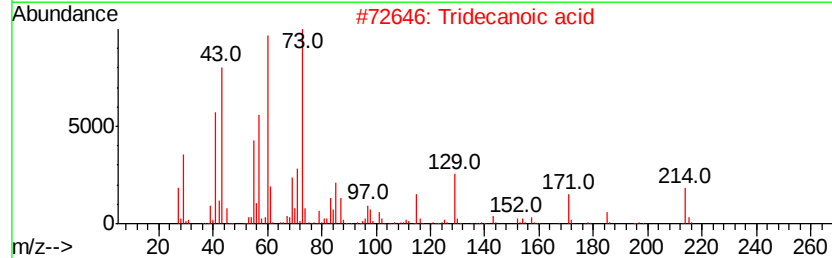
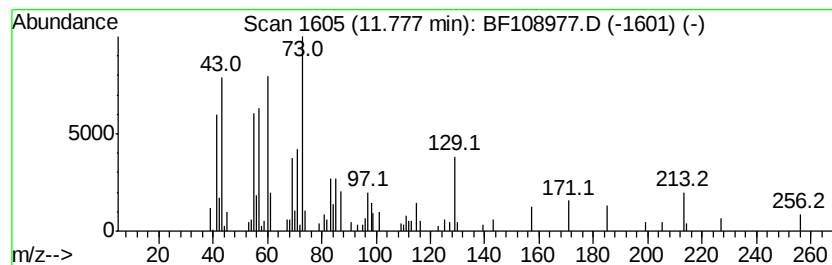
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.78	2.52 ng	133490	Phenanthrene-d10	11.24

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Tridecanoic acid	214	C13H26O2	000638-53-9	90
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5		N-Cyclooct-4-enylacetamide	167	C10H17NO	170952-69-9	25



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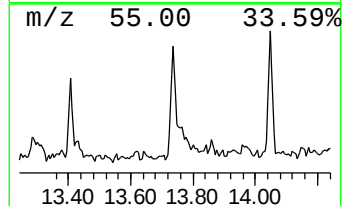
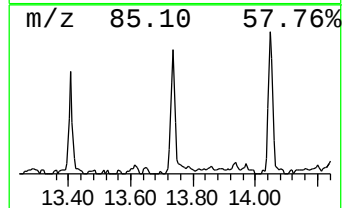
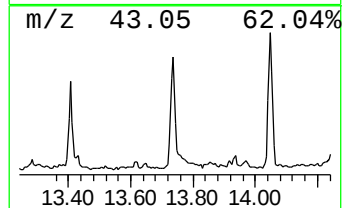
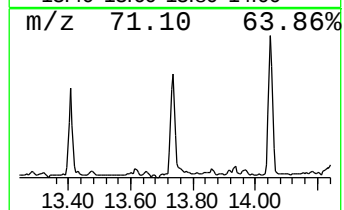
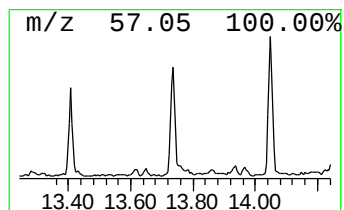
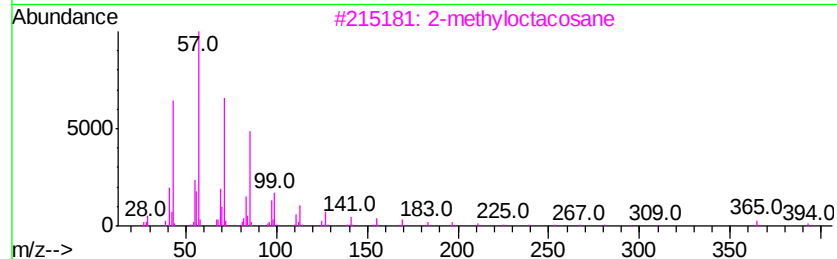
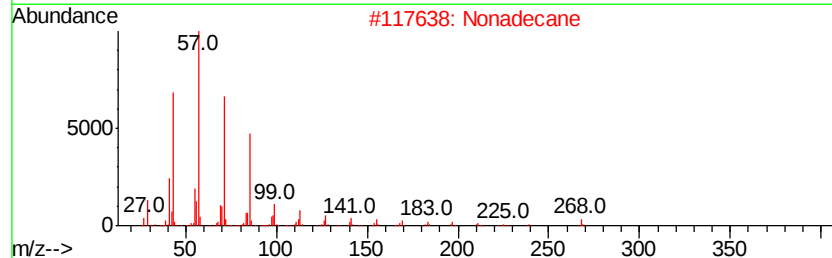
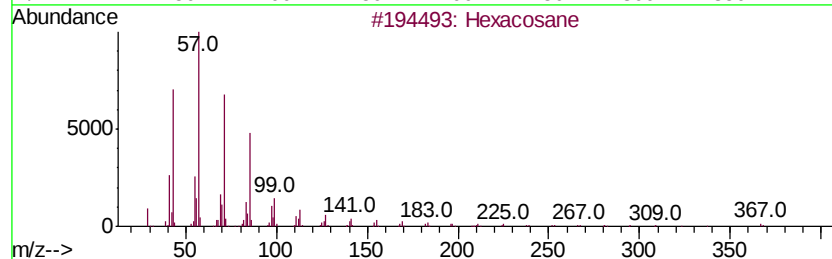
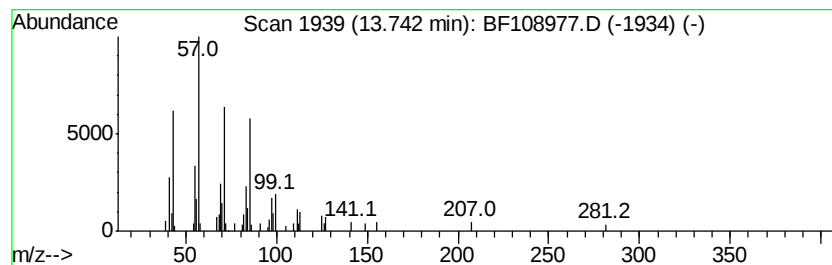
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Hexacosane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.74	2.50 ng	121802	Chrysene-d12	13.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	91
2		Nonadecane	268	C19H40	000629-92-5	86
3		2-methyloctacosane	408	C29H60	1000376-72-8	83
4		Heptacosane	380	C27H56	000593-49-7	74
5		Heneicosane	296	C21H44	000629-94-7	74



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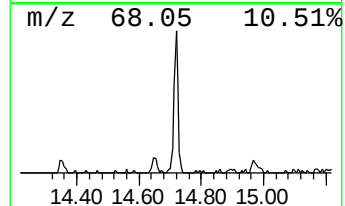
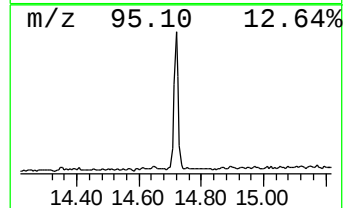
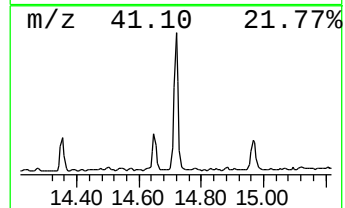
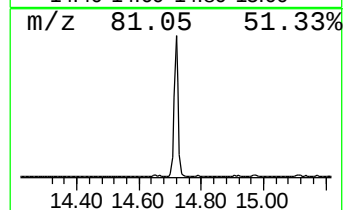
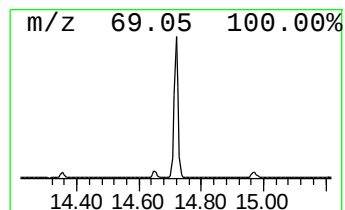
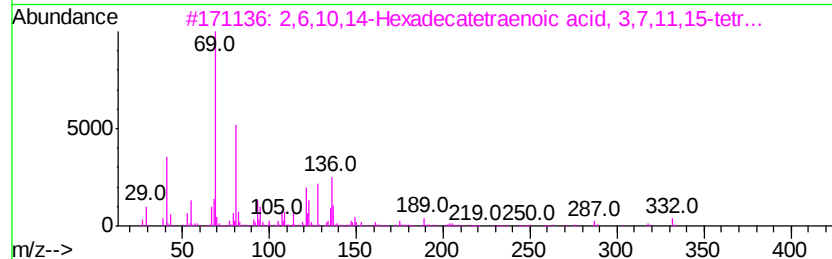
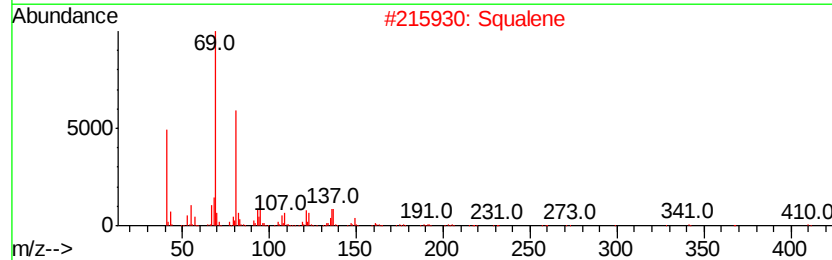
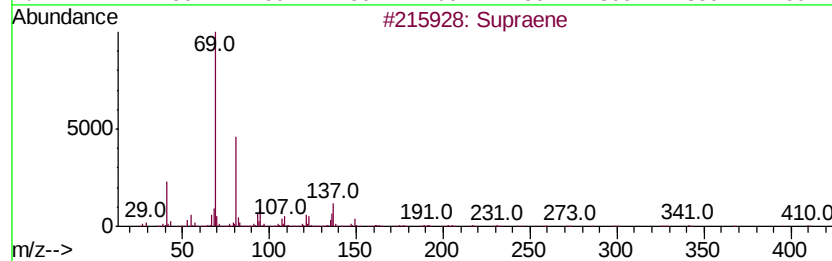
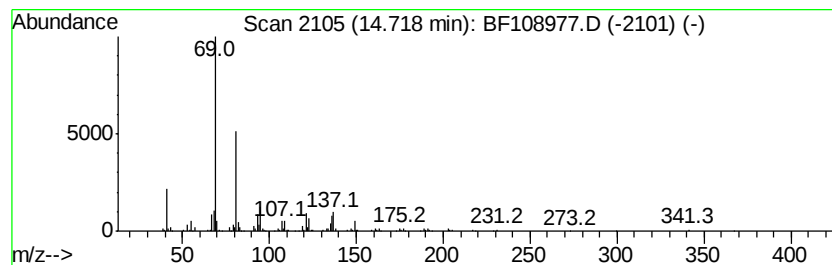
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Supraene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.72	8.69 ng	449389	Perylene-d12	15.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Supraene	410	C30H50	007683-64-9	91
2		Squalene	410	C30H50	000111-02-4	91
3		2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	72
4		(.+/-)-Lavandulol, pentafluorop...	300	C13H17F5O2	1000352-63-1	64
5		2,3,5-Trimethyl-2,3,5-hexanetric...	203	C12H17N3	003974-79-6	50



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091118-DBRI-F-D-B

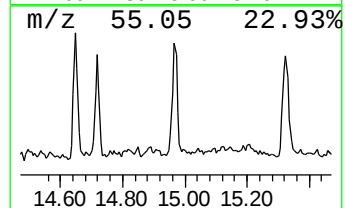
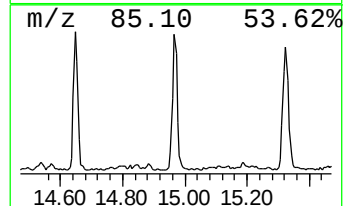
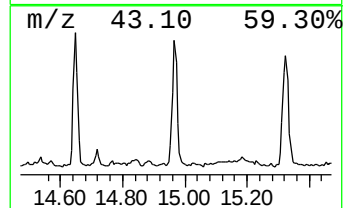
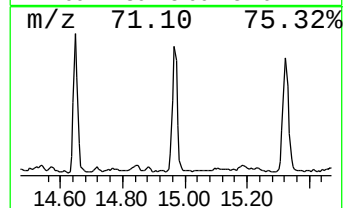
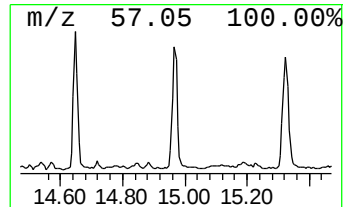
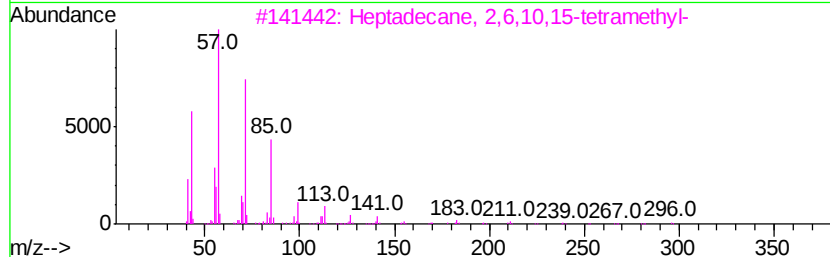
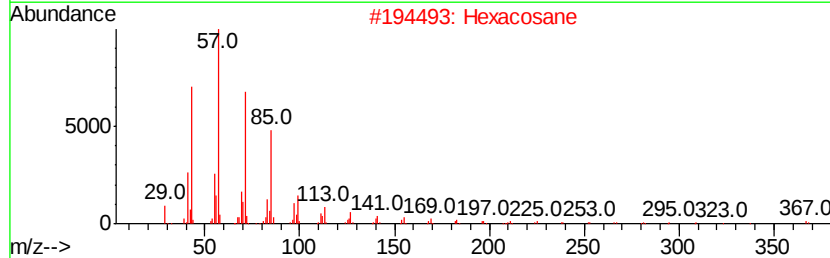
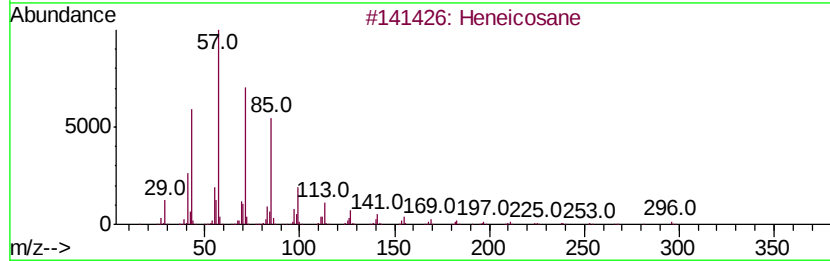
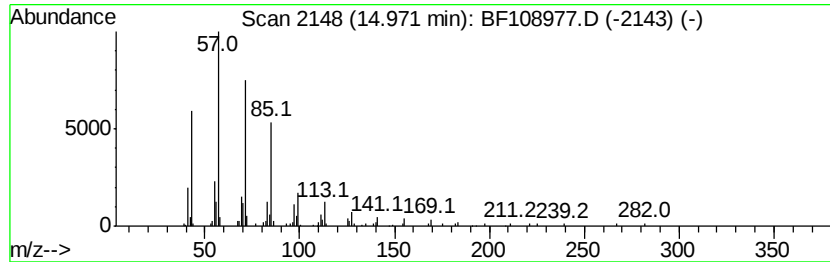
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.97	3.91 ng	202393	Perylene-d12	15.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	91
2		Hexacosane	366	C26H54	000630-01-3	90
3		Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	87
4		Dodecane, 1-iodo-	296	C12H25I	004292-19-7	80
5		Tetracosane	338	C24H50	000646-31-1	68



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF091318\
Data File : BF108977.D
Acq On : 13 Sep 2018 21:04
Operator : JU/SJ
Sample : J4875-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
091118-DBRI-F-D-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.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...	4.91	3.7	ng	157474	1	6.73	849842	20.0
unknown6.50	6.50	58.3	ng	2476070	1	6.73	849842	20.0
n-Hexadecanoic acid	11.78	2.5	ng	133490	4	11.24	1059620	20.0
Hexacosane	13.74	2.5	ng	121802	5	13.86	973566	20.0
Supraene	14.72	8.7	ng	449389	6	15.27	1034680	20.0
Heneicosane	14.97	3.9	ng	202393	6	15.27	1034680	20.0