

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF092618\
 Data File : BF109333.D
 Acq On : 26 Sep 2018 13:51
 Operator : JU/SJ
 Sample : J5059-01
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PHASE-2

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	4.898	474	478	485	rBV	106539	136405	5.87%	0.571%
2	5.316	545	549	553	rBV	1914625	1930282	83.12%	8.083%
3	6.345	719	724	739	rVB	2163080	2132068	91.81%	8.928%
4	6.475	742	746	749	rBV	2352641	2055634	88.52%	8.608%
5	6.540	754	757	765	rBV2	38681	39328	1.69%	0.165%
6	6.704	782	785	789	rBV	871840	689231	29.68%	2.886%
7	6.863	808	812	815	rBV	1980229	1610765	69.37%	6.745%
8	7.263	875	880	883	rBV	1369792	1349353	58.11%	5.651%
9	7.986	999	1003	1006	rBV	1075214	887342	38.21%	3.716%
10	8.704	1121	1125	1133	rBV2	33313	34379	1.48%	0.144%
11	9.063	1181	1186	1189	rBV	2744272	2322154	100.00%	9.724%
12	9.192	1204	1208	1211	rVB	644392	580252	24.99%	2.430%
13	9.457	1249	1253	1256	rBV	598176	465495	20.05%	1.949%
14	9.739	1296	1301	1304	rBV	1043069	1014914	43.71%	4.250%
15	10.328	1397	1401	1411	rBV	396143	372667	16.05%	1.561%
16	10.522	1429	1434	1440	rBV	1684067	1540994	66.36%	6.453%
17	11.216	1548	1552	1554	rBV	1243527	1081467	46.57%	4.529%
18	11.233	1554	1555	1559	rVB	51767	36615	1.58%	0.153%
19	11.410	1581	1585	1589	rBV	44189	47681	2.05%	0.200%
20	11.751	1639	1643	1652	rBV3	157495	189587	8.16%	0.794%
21	12.421	1753	1757	1760	rBV	89326	85733	3.69%	0.359%
22	12.469	1761	1765	1768	rBV	114141	93097	4.01%	0.390%
23	12.533	1773	1776	1781	rBV2	41597	48625	2.09%	0.204%
24	12.645	1789	1795	1798	rBV	87974	95121	4.10%	0.398%
25	12.798	1817	1821	1824	rBV	2592507	2308812	99.43%	9.668%
26	13.039	1856	1862	1865	rBV4	39367	47262	2.04%	0.198%
27	13.251	1895	1898	1901	rBV2	32413	34069	1.47%	0.143%
28	13.380	1917	1920	1923	rBV2	34017	34249	1.47%	0.143%
29	13.498	1934	1940	1944	rBV5	15735	29393	1.27%	0.123%
30	13.710	1972	1976	1983	rVB	71579	94157	4.05%	0.394%
31	13.839	1993	1998	2001	rBV	1068629	961774	41.42%	4.028%
32	14.021	2026	2029	2032	rVB2	32523	30226	1.30%	0.127%
33	14.327	2078	2081	2083	rBV	32290	31473	1.36%	0.132%
34	14.621	2128	2131	2135	rVB	45687	42765	1.84%	0.179%

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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	14.686	2139	2142	2148	rVB	111691	109870	4.73%	0.460%
36	14.845	2165	2169	2172	rBV	37754	52577	2.26%	0.220%
37	14.933	2181	2184	2190	rVB2	62896	70643	3.04%	0.296%
38	15.180	2222	2226	2229	rVB	30530	34581	1.49%	0.145%
39	15.239	2231	2236	2240	rBV	722996	823936	35.48%	3.450%
40	15.286	2240	2244	2249	rVB2	75265	99820	4.30%	0.418%
41	15.692	2308	2313	2318	rBV	63521	93487	4.03%	0.391%
42	16.151	2387	2391	2400	rVB2	43203	79678	3.43%	0.334%
43	16.692	2479	2483	2489	rVB4	19224	35681	1.54%	0.149%
44	16.992	2529	2534	2538	rBV4	13437	26406	1.14%	0.111%

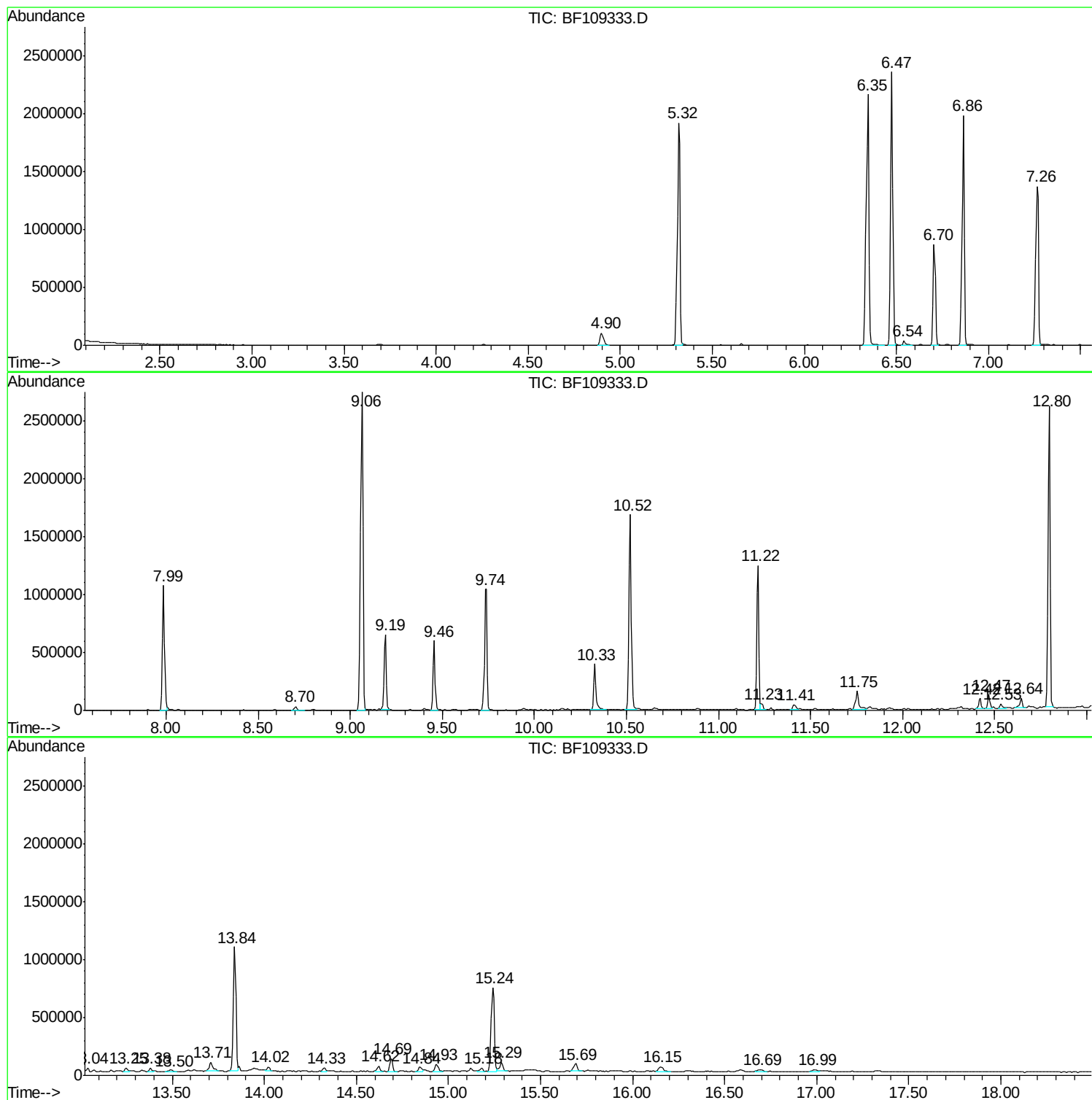
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF092218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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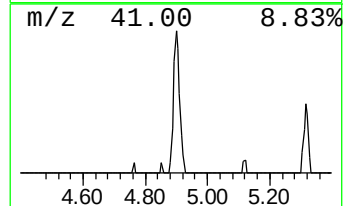
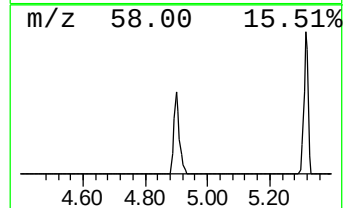
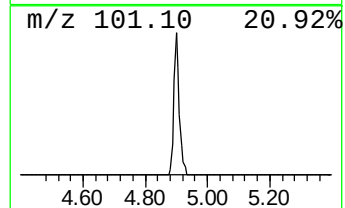
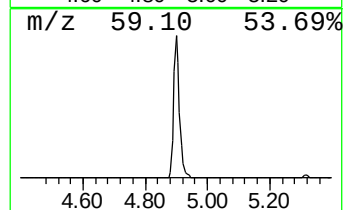
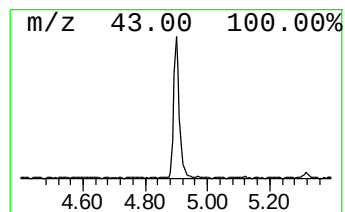
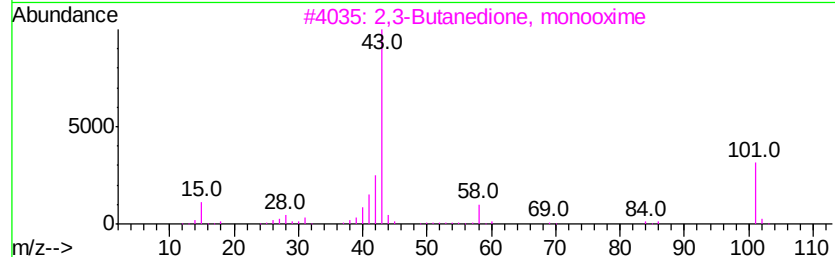
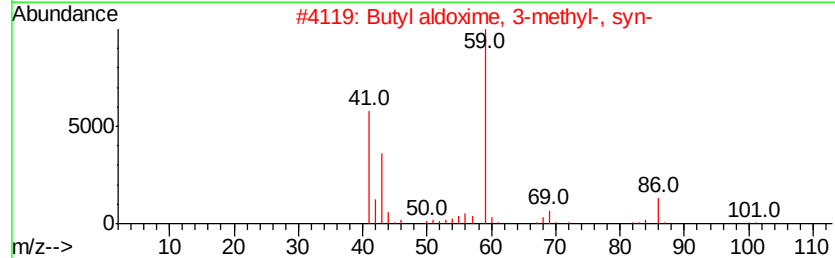
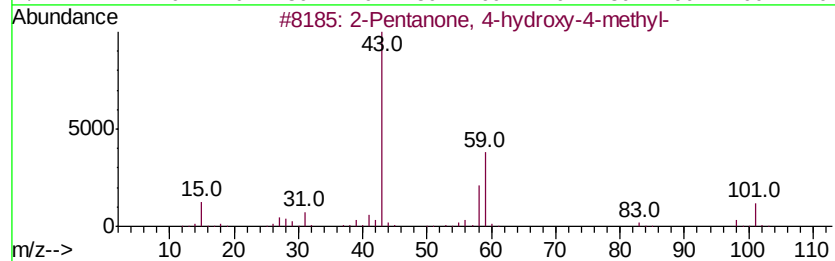
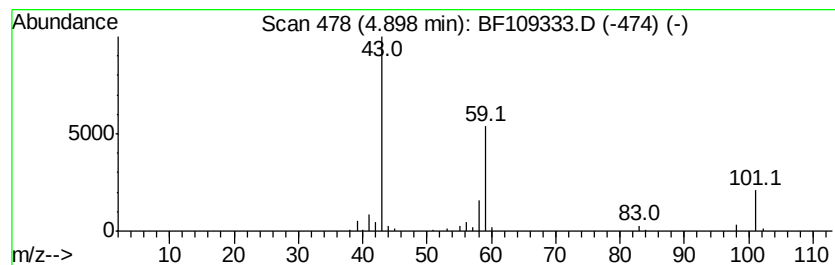
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF092218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.90	3.96 ng	136405	1,4-Dichlorobenzene-d4	6.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	47
2		Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	17
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		5-Hexen-2-one	98	C6H10O	000109-49-9	9



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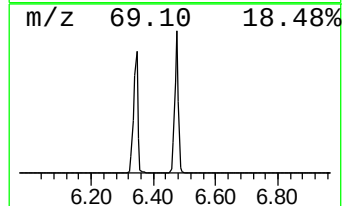
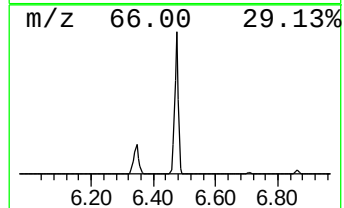
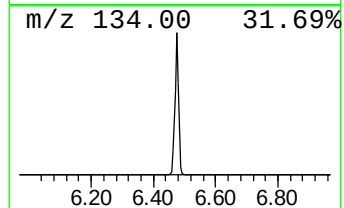
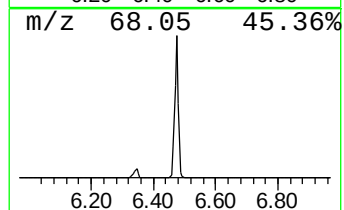
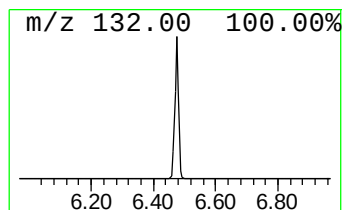
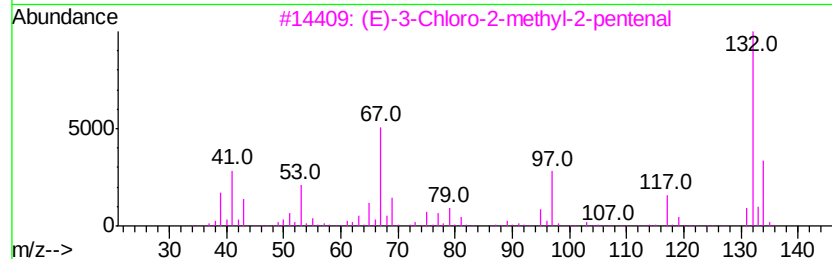
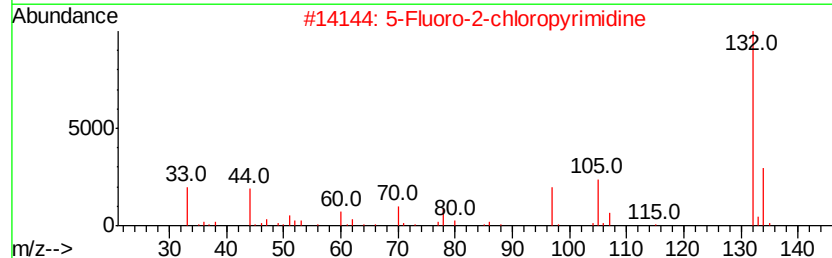
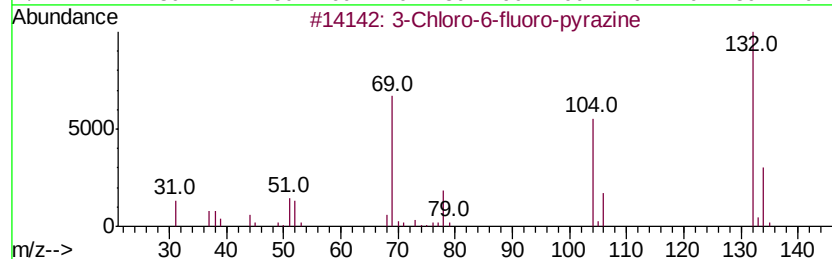
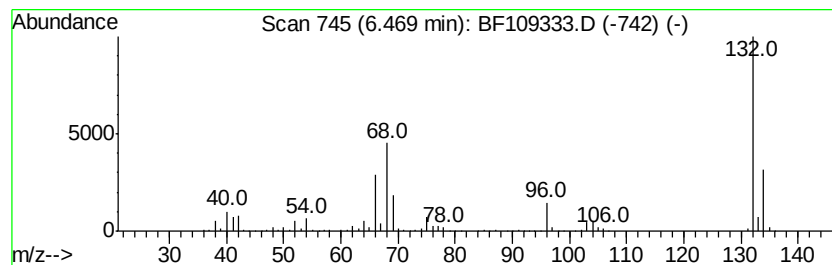
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Peak Number 2 unknown6.47 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.47	59.65 ng	2055630	1,4-Dichlorobenzene-d4	6.70

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		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
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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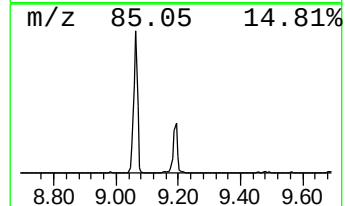
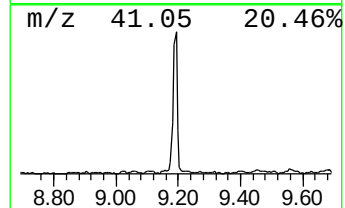
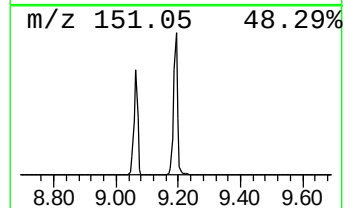
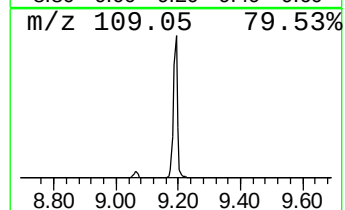
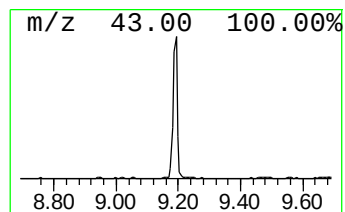
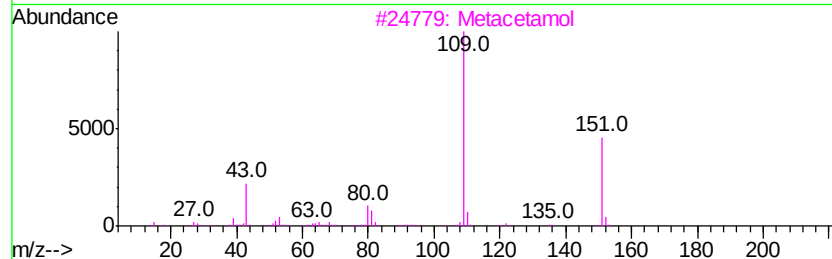
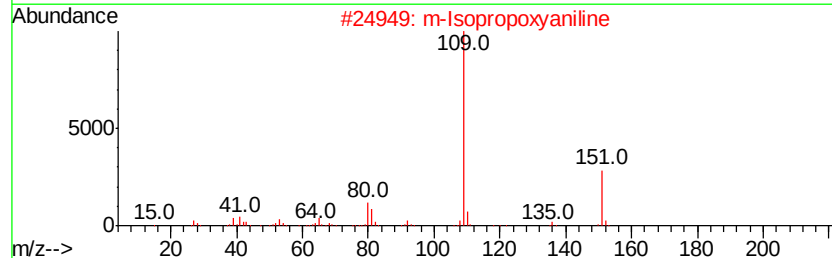
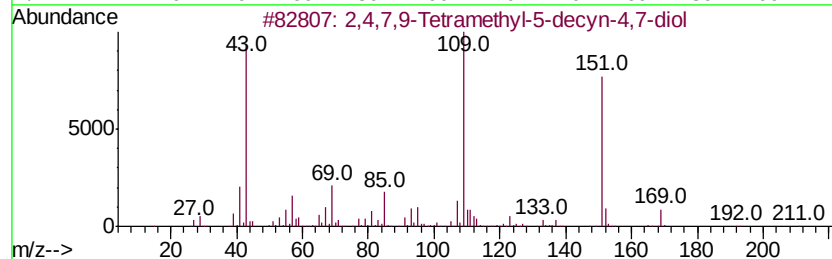
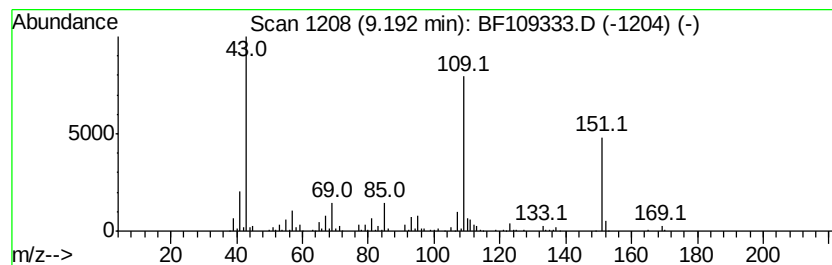
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.19	11.43 ng	580252	Acenaphthene-d10	9.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	91
2		m-Isopropoxyaniline	151	C9H13NO	041406-00-2	59
3		Metacetamol	151	C8H9NO2	000621-42-1	59
4		Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	59
5		Acetaminophen	151	C8H9NO2	000103-90-2	59



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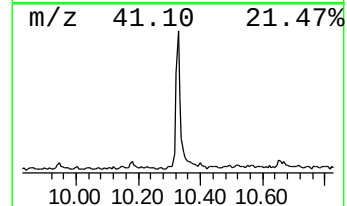
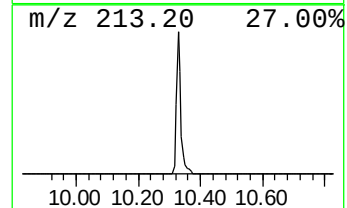
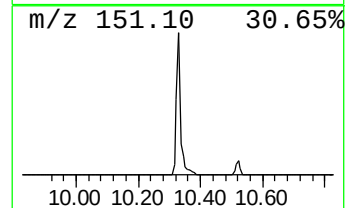
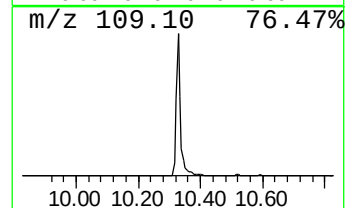
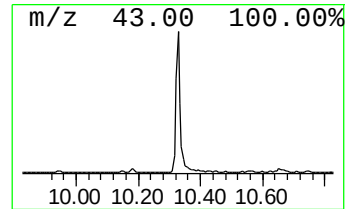
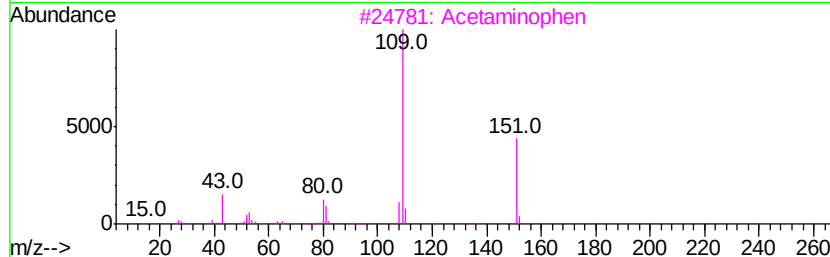
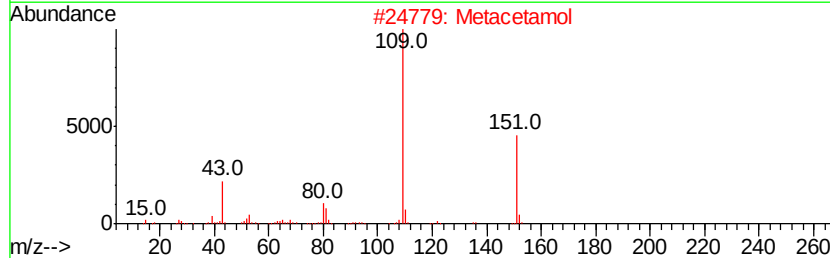
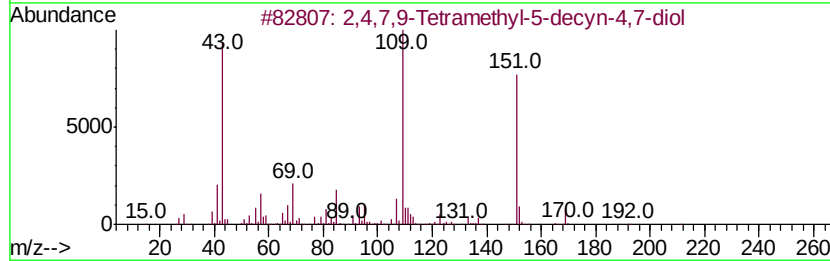
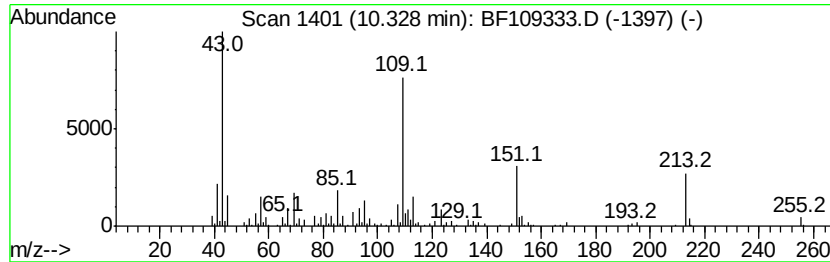
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 unknown10.33 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.33	7.34 ng	372667	Acenaphthene-d10	9.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2		000126-86-3	68
2	Metacetamol	151	C8H9NO2		000621-42-1	46
3	Acetaminophen	151	C8H9NO2		000103-90-2	46
4	4-Pyridinemethanol, acetate (ester)	151	C8H9NO2		001007-48-3	43
5	m-Isopropoxyaniline	151	C9H13NO		041406-00-2	43



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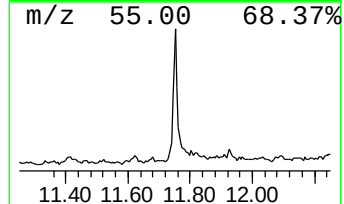
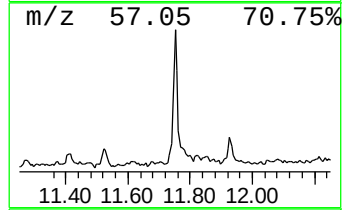
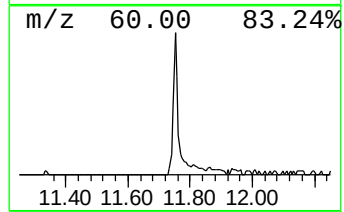
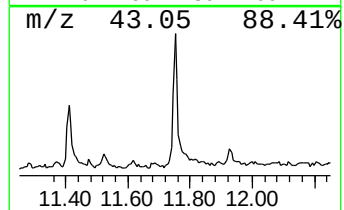
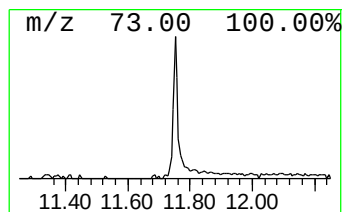
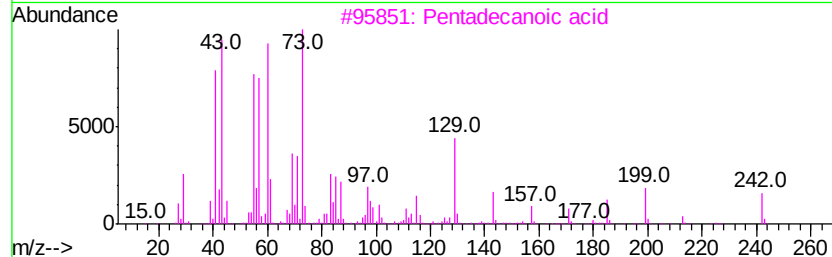
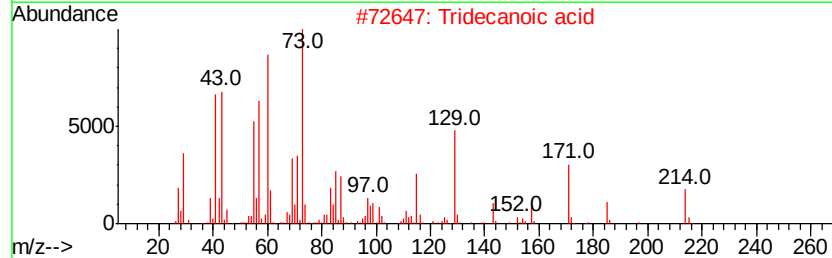
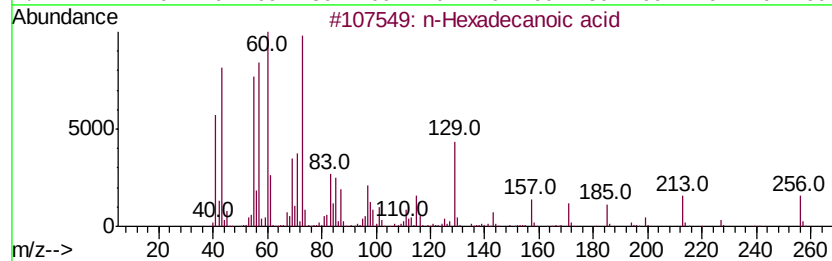
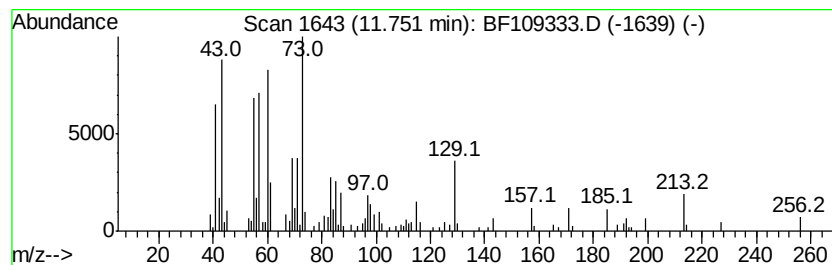
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.75	3.51 ng	189587	Phenanthrene-d10	11.22

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tridecanoic acid	214	C13H26O2	000638-53-9	95
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5		Dodecanoic acid	200	C12H24O2	000143-07-7	53



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF092618\
Data File : BF109333.D
Acq On : 26 Sep 2018 13:51
Operator : JU/SJ
Sample : J5059-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

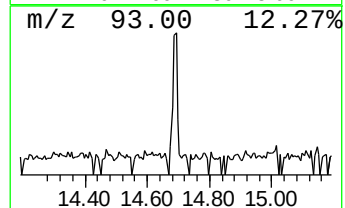
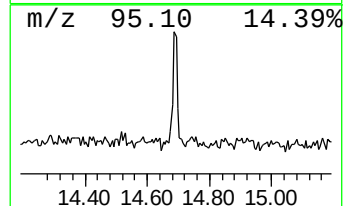
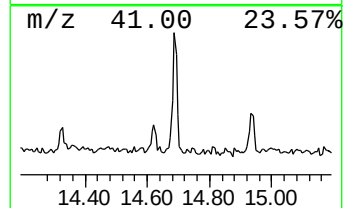
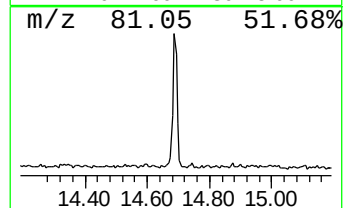
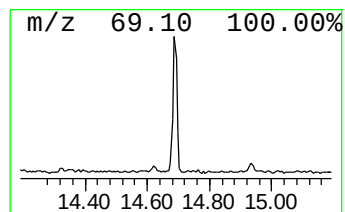
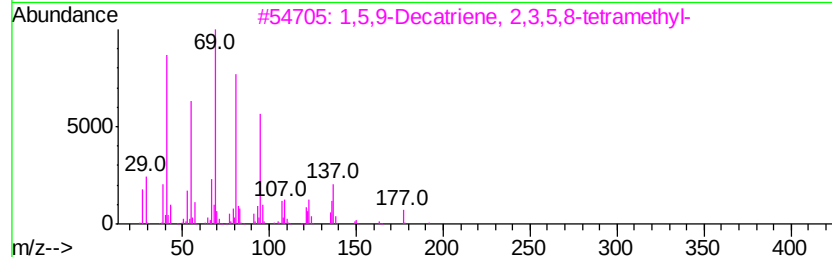
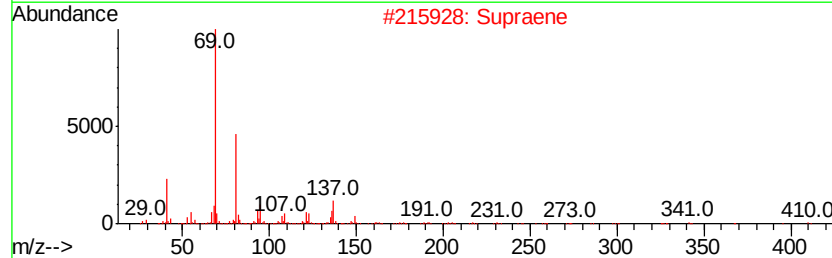
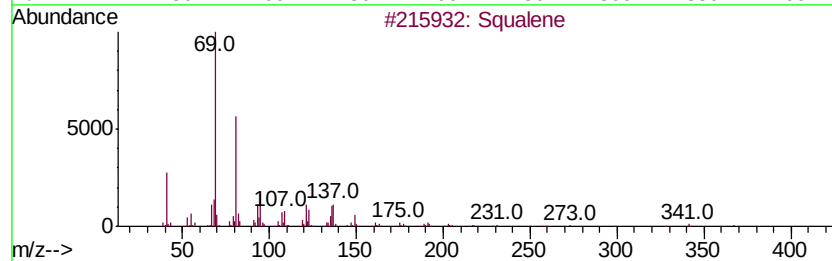
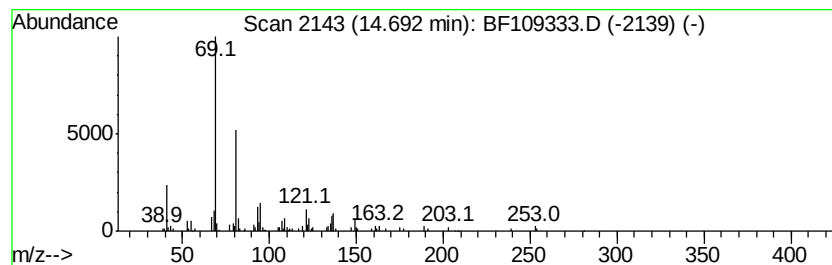
Instrument :
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ClientSampleId :
PHASE-2

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 7 Squalene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.69	2.67 ng	109870	Perylene-d12	15.24
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Squalene	410 C30H50	000111-02-4	91
2	Supraene	410 C30H50	007683-64-9	90
3	1,5,9-Decatriene, 2,3,5,8-tetram...	192 C14H24	230646-72-7	64
4	3-Cyclohexene-1-carboxaldehyde, ...	192 C13H20O	052475-89-5	59
5	1,5-Heptadiene, 3,3,6-trimethyl-	138 C10H18	035387-63-4	58



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF092618\
Data File : BF109333.D
Acq On : 26 Sep 2018 13:51
Operator : JU/SJ
Sample : J5059-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PHASE-2

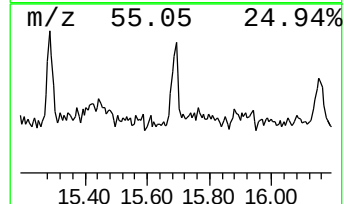
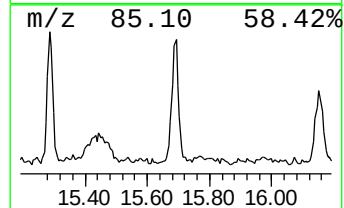
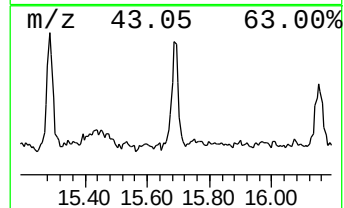
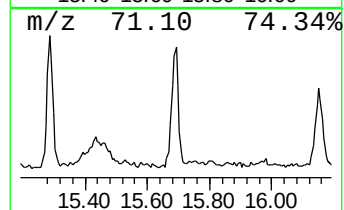
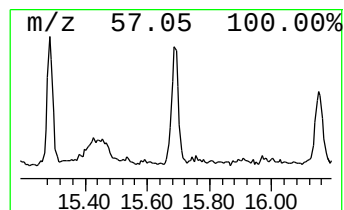
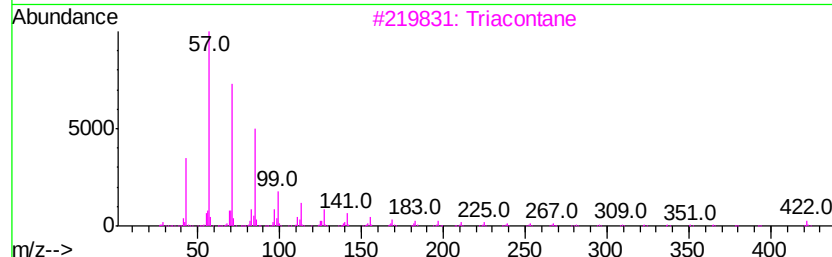
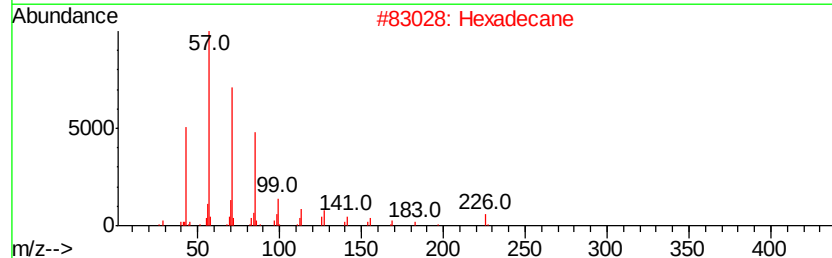
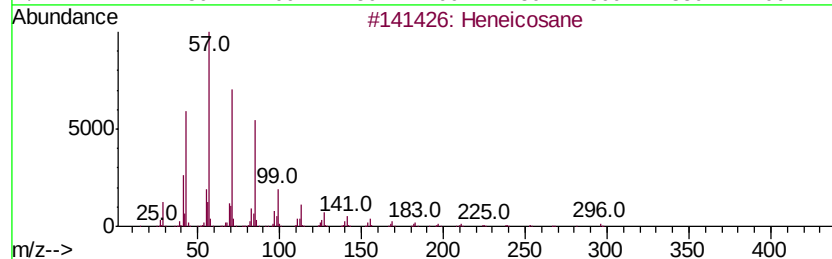
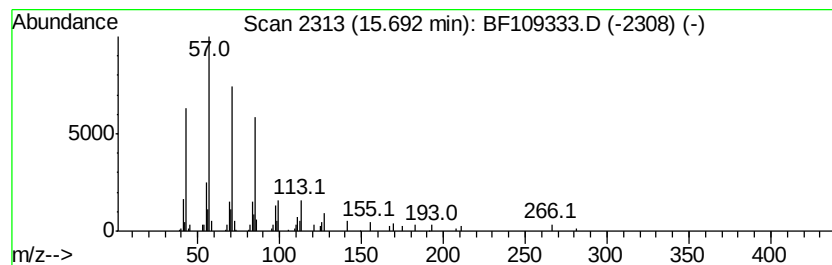
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.69	2.27 ng	93487	Perylene-d12	15.24

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	91
2	Hexadecane		226	C16H34	000544-76-3	90
3	Triacontane		422	C30H62	000638-68-6	90
4	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	90
5	Hexacosane		366	C26H54	000630-01-3	87



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Data File : BF109333.D
Acq On : 26 Sep 2018 13:51
Operator : JU/SJ
Sample : J5059-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PHASE-2

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	4.0	ng	136405	1	6.70	689231	20.0
unknown6.47	6.47	59.6	ng	2055630	1	6.70	689231	20.0
2,4,7,9-Tetrameth...	9.19	11.4	ng	580252	3	9.73	1014910	20.0
unknown10.33	10.33	7.3	ng	372667	3	9.73	1014910	20.0
n-Hexadecanoic acid	11.75	3.5	ng	189587	4	11.22	1081470	20.0
Squalene	14.69	2.7	ng	109870	6	15.24	823936	20.0
Heneicosane	15.69	2.3	ng	93487	6	15.24	823936	20.0