

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF072618\
 Data File : BF107709.D
 Acq On : 26 Jul 2018 19:32
 Operator : JU/SJ
 Sample : J4095-13
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CON-SB-104-05-06-07-0-11

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-BF072018.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	5.195	482	486	495	rBV	277280	394826	11.13%	1.171%
2	5.595	551	554	575	rBV	1403059	2622630	73.96%	7.777%
3	6.595	721	724	744	rBV	1601163	3014504	85.01%	8.939%
4	6.736	744	748	774	rVB	2297319	3264472	92.06%	9.680%
5	6.960	783	786	804	rVB	599469	943407	26.60%	2.798%
6	7.113	809	812	840	rVB	1984768	2436044	68.70%	7.224%
7	7.525	878	882	906	rBV	1286213	2034071	57.36%	6.032%
8	7.678	906	908	918	rVB2	29832	45846	1.29%	0.136%
9	8.242	1000	1004	1023	rBV	1026741	1396600	39.38%	4.141%
10	9.313	1182	1186	1202	rBV	3153715	3546162	100.00%	10.516%
11	9.707	1249	1253	1265	rBV	217102	236368	6.67%	0.701%
12	10.001	1299	1303	1322	rVB	1490857	1560151	44.00%	4.626%
13	10.383	1364	1368	1371	rBV2	32091	43342	1.22%	0.129%
14	10.795	1434	1438	1451	rBV	1985809	2459490	69.36%	7.293%
15	10.883	1451	1453	1459	rVB3	32997	54270	1.53%	0.161%
16	11.495	1553	1557	1569	rBV2	1348618	1844016	52.00%	5.468%
17	11.760	1597	1602	1605	rBV4	31962	41011	1.16%	0.122%
18	12.001	1639	1643	1646	rBV	173573	197838	5.58%	0.587%
19	12.113	1659	1662	1664	rBV3	39828	37527	1.06%	0.111%
20	12.171	1669	1672	1675	rBV2	30494	36769	1.04%	0.109%
21	12.324	1695	1698	1703	rBV6	30398	53633	1.51%	0.159%
22	12.448	1716	1719	1721	rBV2	38712	39277	1.11%	0.116%
23	12.554	1734	1737	1740	rBV3	48609	54922	1.55%	0.163%
24	12.713	1758	1764	1768	rBV	334687	423892	11.95%	1.257%
25	12.871	1788	1791	1794	rVB	150331	114243	3.22%	0.339%
26	12.942	1798	1803	1810	rVV	269546	404330	11.40%	1.199%
27	13.077	1822	1826	1833	rBV	2815037	2746500	77.45%	8.144%
28	13.283	1859	1861	1864	rVB	78254	71679	2.02%	0.213%
29	13.313	1864	1866	1873	rBV3	42805	70129	1.98%	0.208%
30	13.407	1880	1882	1892	rVB3	54428	102380	2.89%	0.304%
31	13.624	1917	1919	1922	rBV2	53334	57876	1.63%	0.172%
32	13.954	1972	1975	1978	rBV3	167625	177339	5.00%	0.526%
33	14.142	2003	2007	2011	rBV	917139	1145645	32.31%	3.397%
34	14.748	2107	2110	2114	rVB	186043	191473	5.40%	0.568%

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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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.895	2133	2135	2141	rVB2	99867	109904	3.10%	0.326%
36	15.218	2187	2190	2193	rBV	95808	144515	4.08%	0.429%
37	15.607	2253	2256	2261	rBV	100155	148687	4.19%	0.441%
38	15.677	2261	2268	2282	rVB	724728	1337874	37.73%	3.967%
39	16.112	2339	2342	2347	rVB	75259	119104	3.36%	0.353%

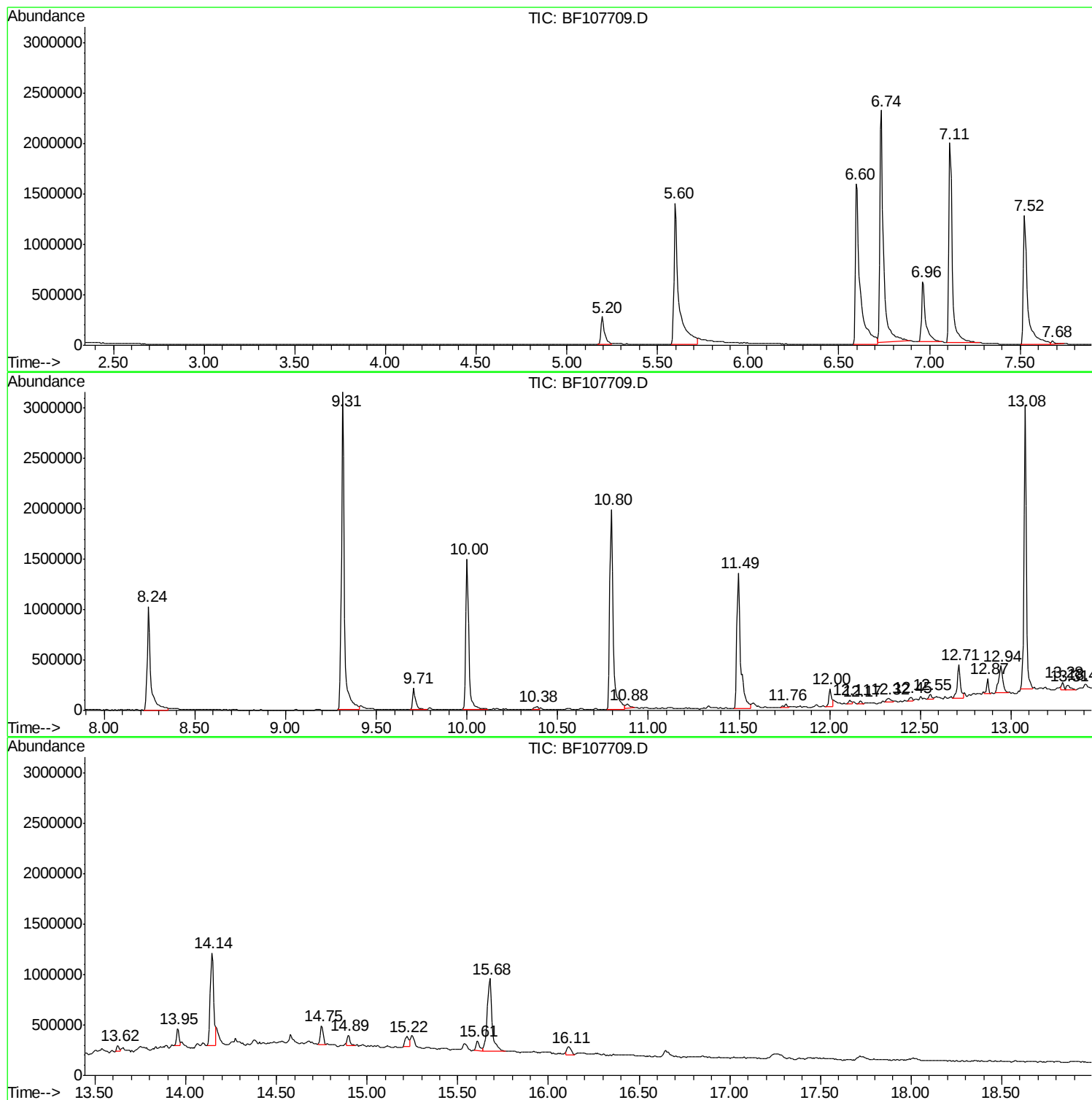
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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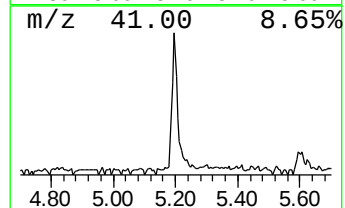
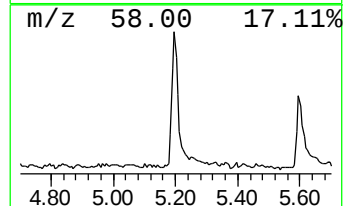
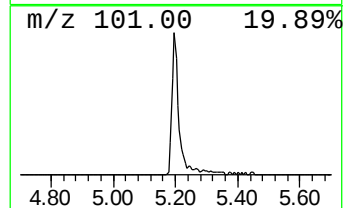
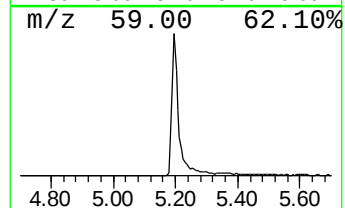
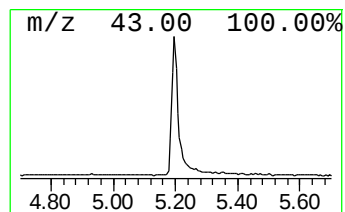
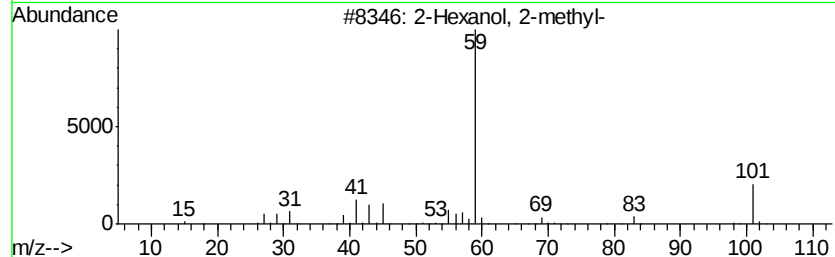
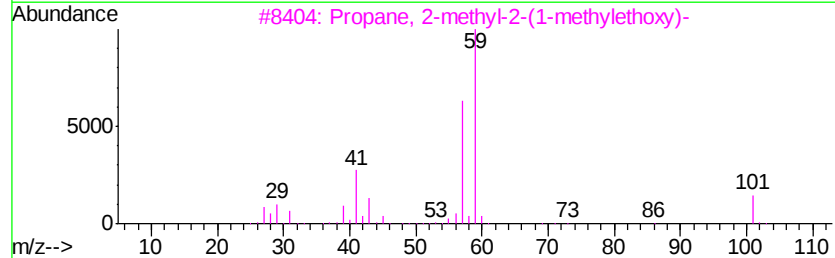
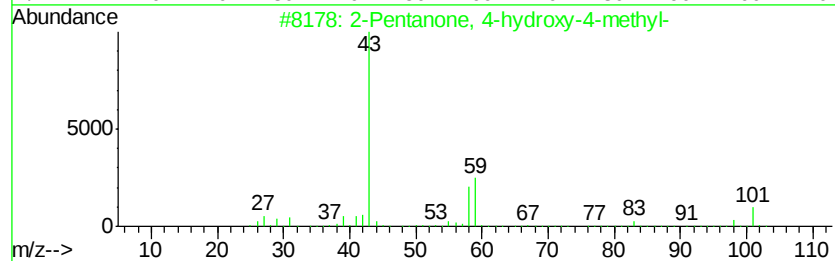
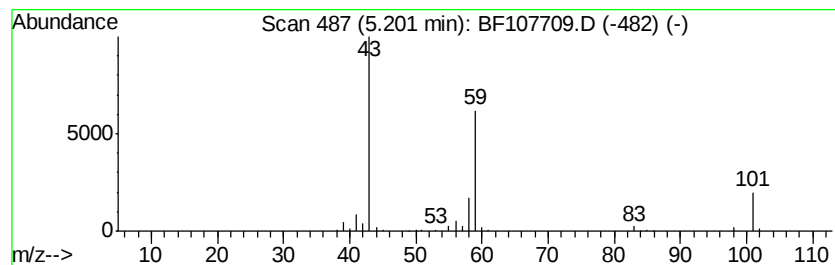
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.20	8.37 ng	394826	1,4-Dichlorobenzene-d4	6.96

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	40
4			3-Octanol	130	C8H18O	000589-98-0	33
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25



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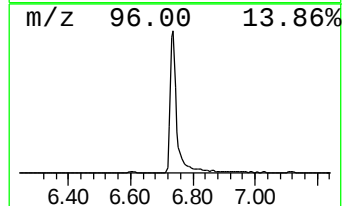
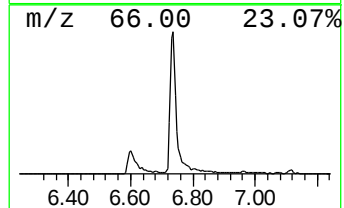
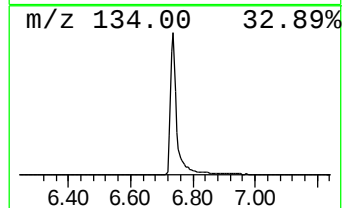
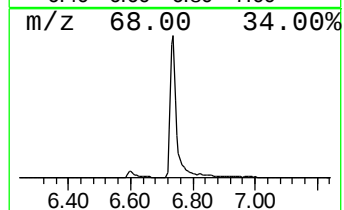
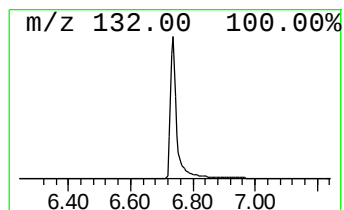
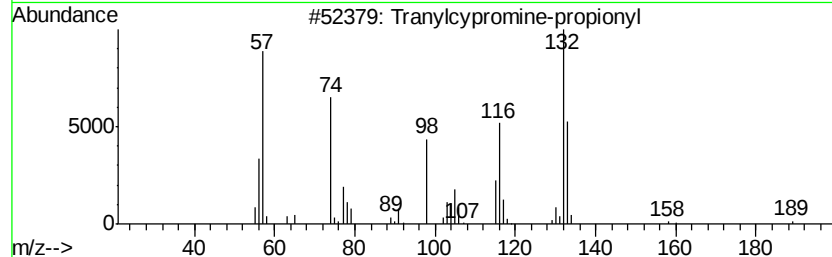
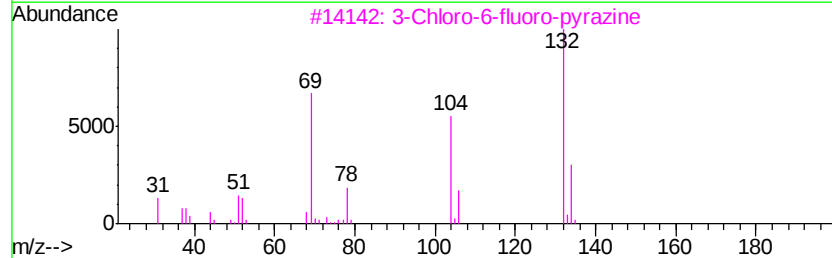
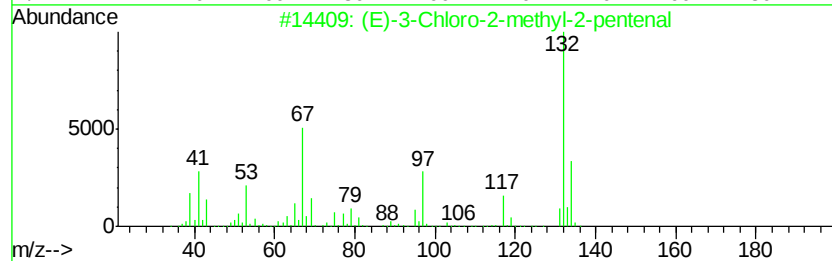
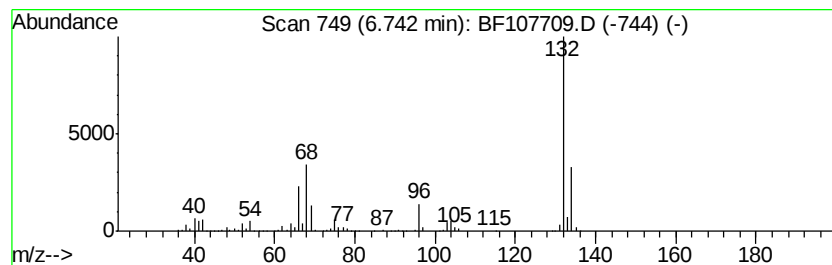
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.74 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	69.21 ng	3264470	1,4-Dichlorobenzene-d4	6.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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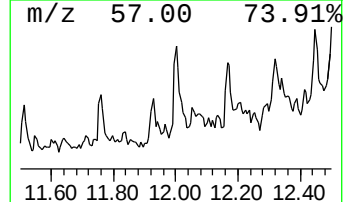
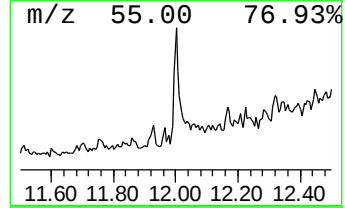
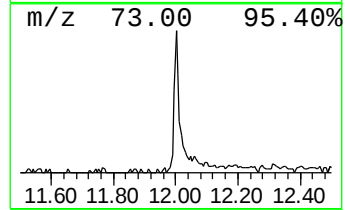
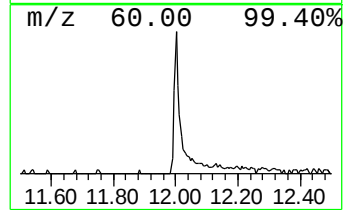
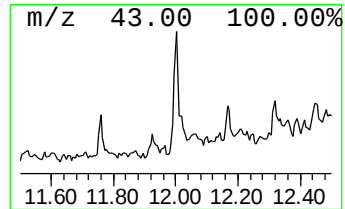
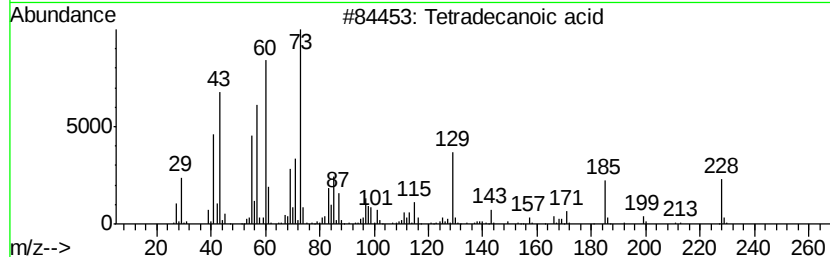
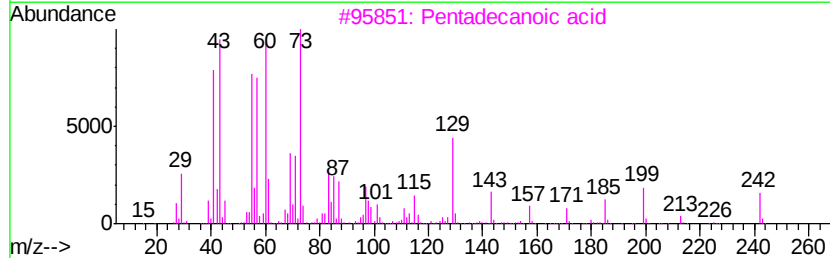
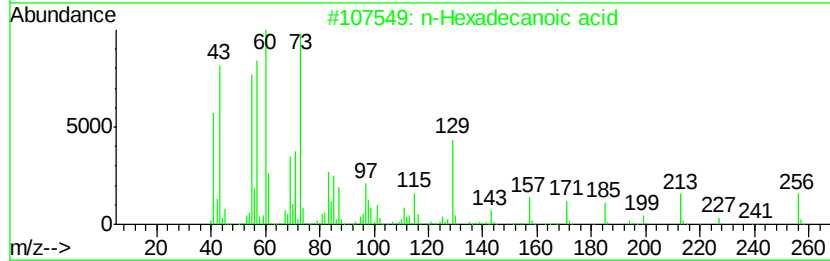
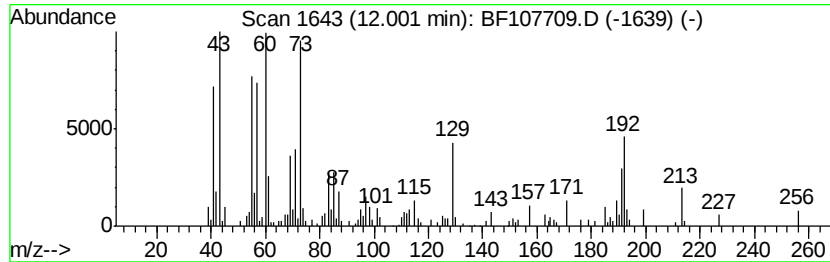
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.00	2.15 ng	197838	Phenanthrene-d10	11.49	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	70
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	62
4	Tridecanoic acid	214	C13H26O2	000638-53-9	60
5	n-Decanoic acid	172	C10H20O2	000334-48-5	49



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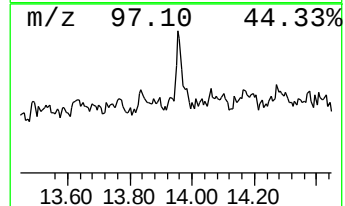
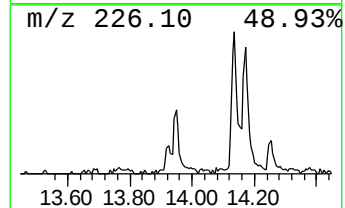
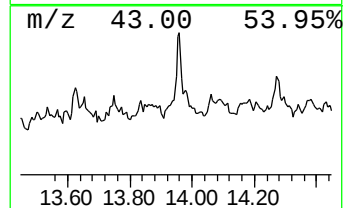
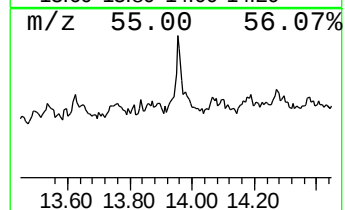
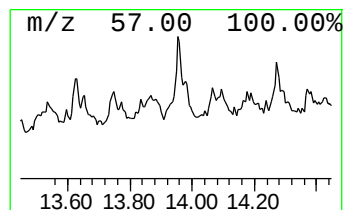
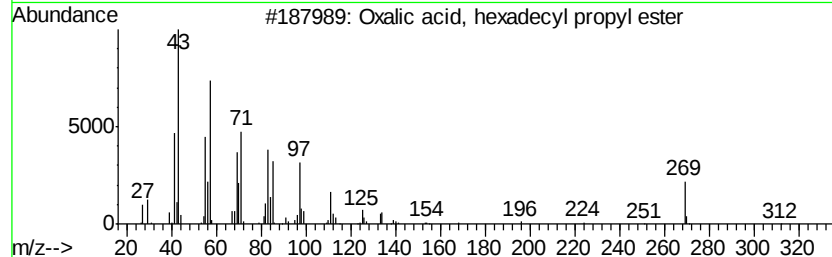
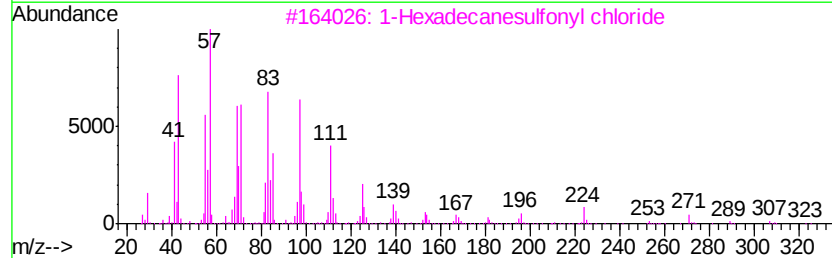
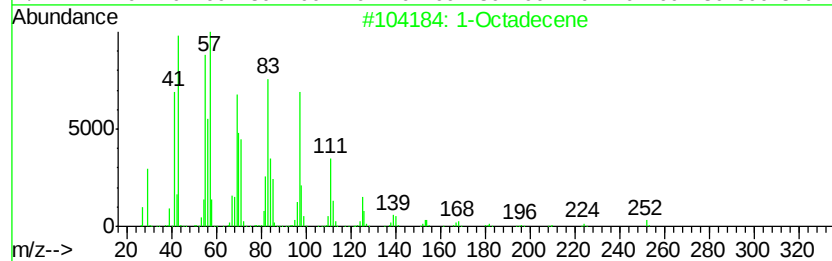
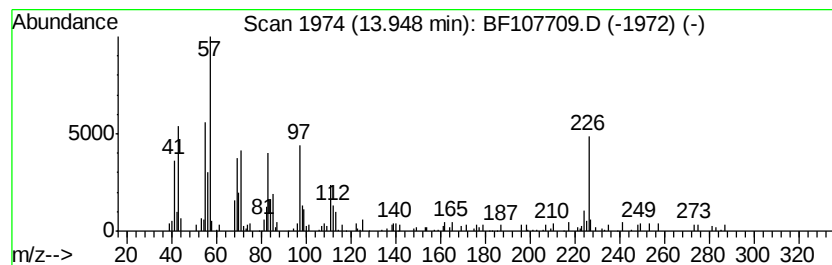
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1-Octadecene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.95	3.10 ng	177339	Chrysene-d12	14.14
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Octadecene	252 C18H36	000112-88-9	96
2	1-Hexadecanesulfonyl chloride	324 C16H33ClO2S	038775-38-1	91
3	Oxalic acid, hexadecyl propyl ester	356 C21H40O4	1000309-26-9	91
4	17-Pentatriacontene	491 C35H70	006971-40-0	91
5	Trichloroacetic acid, tetradecyl...	358 C16H29Cl3O2	074339-52-9	81



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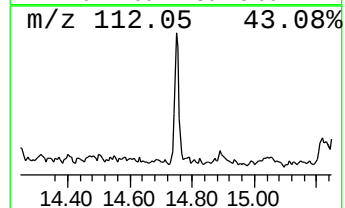
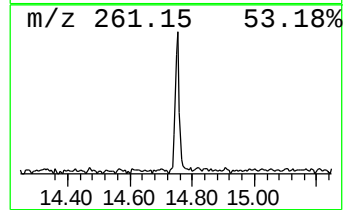
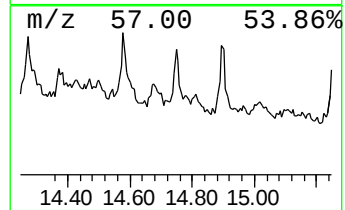
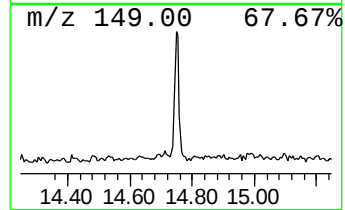
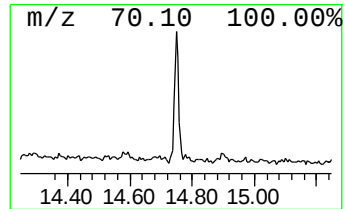
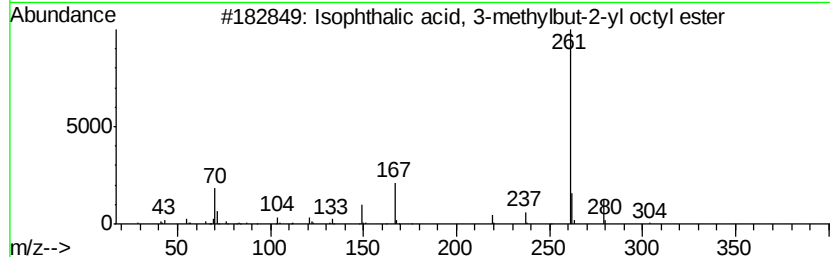
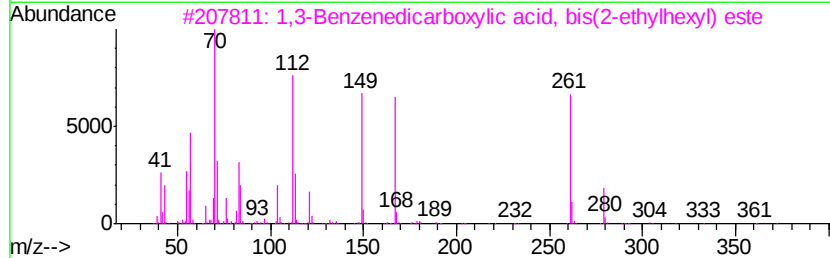
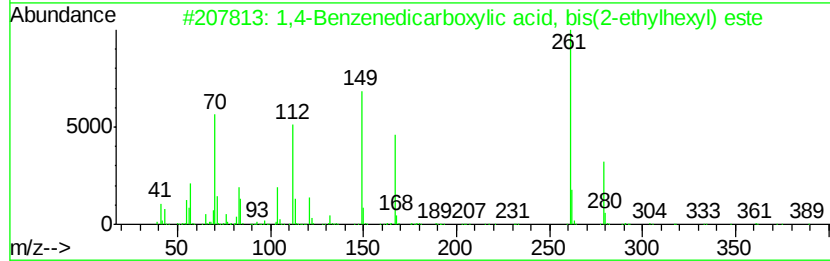
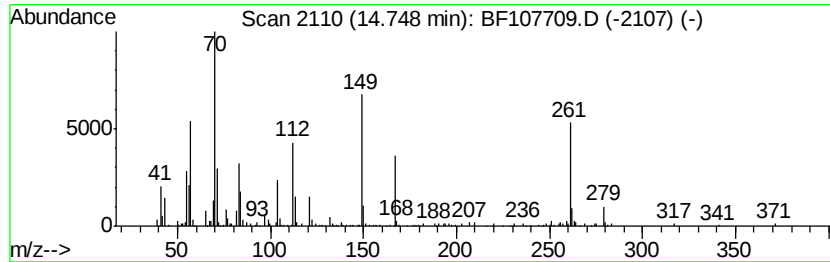
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 1,4-Benzenedicarboxylic aci... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.75	3.34 ng	191473	Chrysene-d12	14.14

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	72
2		1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	52
3		Isophthalic acid, 3-methylbut-2-...	348	C21H32O4	1000344-72-4	50
4		Terephthalic acid, di(4-octyl) e...	390	C24H38O4	1000323-74-2	43
5		Terephthalic acid, monochloride,...	296	C16H21ClO3	1000324-22-9	35



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF072618\
Data File : BF107709.D
Acq On : 26 Jul 2018 19:32
Operator : JU/SJ
Sample : J4095-13
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CON-SB-104-05-06-07-0-11

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.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...	5.20	8.4	ng	394826	1	6.96	943407	20.0
unknown6.74	6.74	69.2	ng	3264470	1	6.96	943407	20.0
n-Hexadecanoic acid	12.00	2.1	ng	197838	4	11.49	1844020	20.0
1-Octadecene	13.95	3.1	ng	177339	5	14.14	1145650	20.0
1,4-Benzenedicarb...	14.75	3.3	ng	191473	5	14.14	1145650	20.0