

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF072718\
 Data File : BF107761.D
 Acq On : 27 Jul 2018 22:10
 Operator : JU/SJ
 Sample : J4112-02
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CON-SB-08-09-0-11

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	5.201	483	487	503	rBV	415161	597743	15.04%	1.735%
2	5.596	550	554	583	rBV	2373580	3527687	88.79%	10.241%
3	6.595	720	724	743	rBV	2253537	3527599	88.79%	10.240%
4	6.737	743	748	771	rVB	2876871	3858740	97.12%	11.202%
5	6.960	783	786	808	rVB	589898	933229	23.49%	2.709%
6	7.113	808	812	838	rBV	2576519	2956050	74.40%	8.581%
7	7.525	878	882	906	rBV	1473036	2323128	58.47%	6.744%
8	8.242	1000	1004	1028	rBV	934868	1202840	30.27%	3.492%
9	9.313	1182	1186	1201	rBV	3620391	3973138	100.00%	11.534%
10	9.707	1249	1253	1262	rBV	298507	309372	7.79%	0.898%
11	10.001	1298	1303	1315	rBV	1047452	1171193	29.48%	3.400%
12	10.795	1434	1438	1451	rBV	1770503	2236501	56.29%	6.492%
13	10.883	1451	1453	1459	rVB4	43205	60790	1.53%	0.176%
14	11.495	1553	1557	1565	rBV	832024	1026621	25.84%	2.980%
15	12.001	1640	1643	1647	rBV	79479	91600	2.31%	0.266%
16	12.713	1761	1764	1768	rBV	75228	80449	2.02%	0.234%
17	12.871	1788	1791	1794	rBV	144356	130297	3.28%	0.378%
18	12.948	1797	1804	1810	rBV2	78621	147393	3.71%	0.428%
19	13.077	1822	1826	1837	rBV	3041444	3147447	79.22%	9.137%
20	13.954	1972	1975	1981	rBV2	130352	147045	3.70%	0.427%
21	14.148	2003	2008	2019	rBV	878073	1270730	31.98%	3.689%
22	14.577	2079	2081	2086	rVB2	80821	80075	2.02%	0.232%
23	14.748	2108	2110	2113	rVB	133711	117425	2.96%	0.341%
24	14.895	2133	2135	2138	rVB	73582	63815	1.61%	0.185%
25	14.977	2146	2149	2153	rVB	87448	97012	2.44%	0.282%
26	15.248	2192	2195	2201	rVB	156276	184429	4.64%	0.535%
27	15.677	2264	2268	2283	rVB	592993	1003280	25.25%	2.912%
28	16.107	2338	2341	2347	rVB	115829	182021	4.58%	0.528%

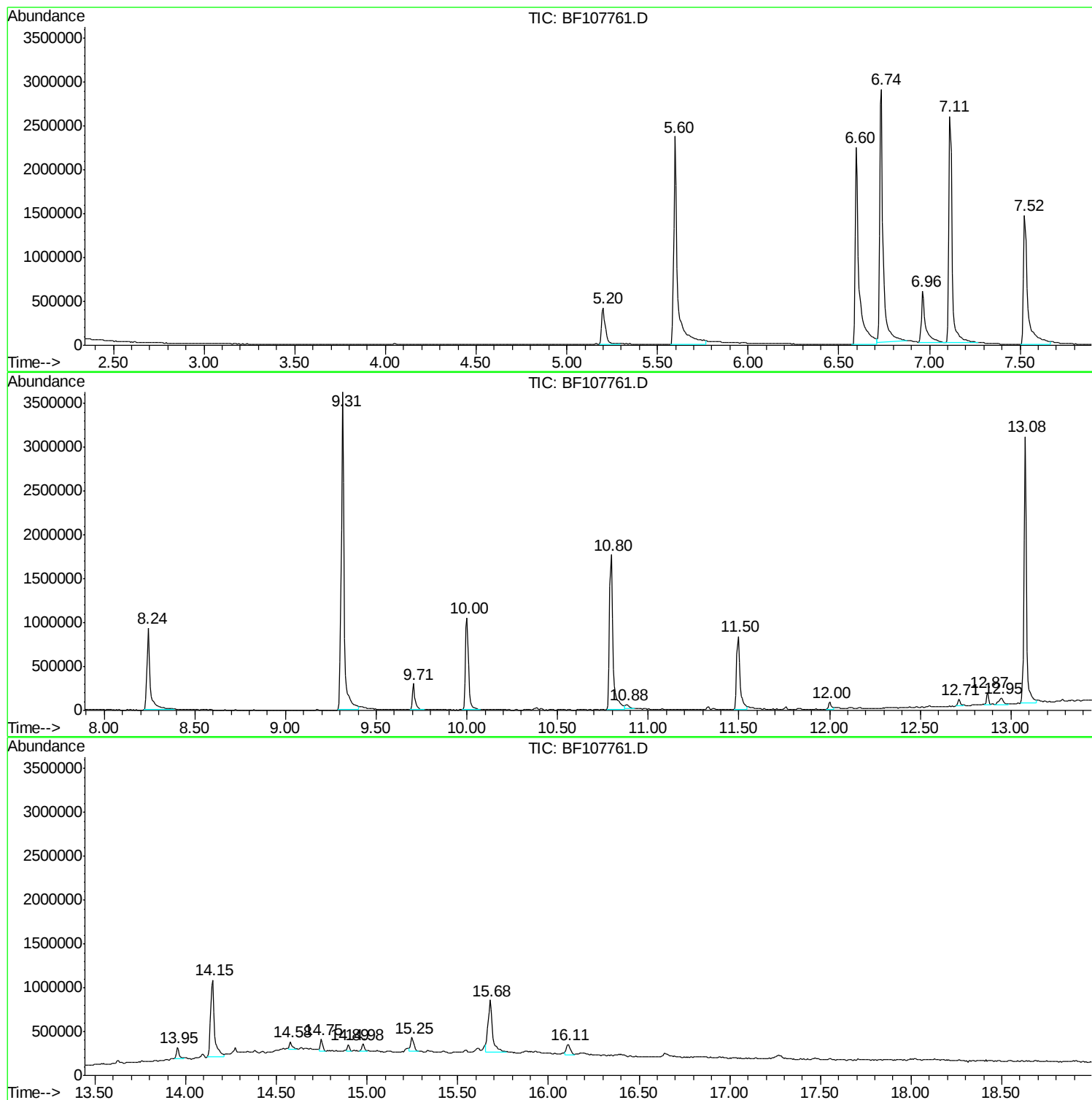
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF072018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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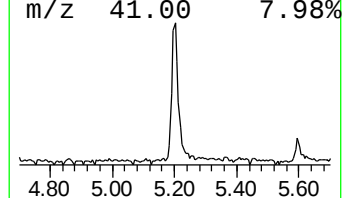
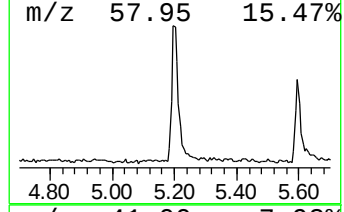
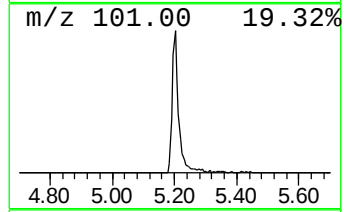
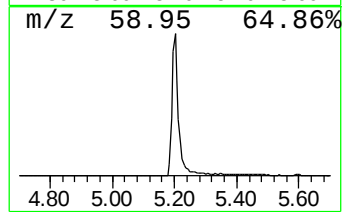
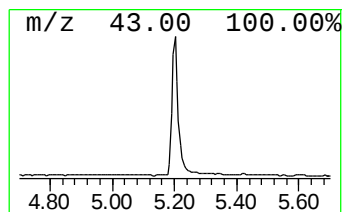
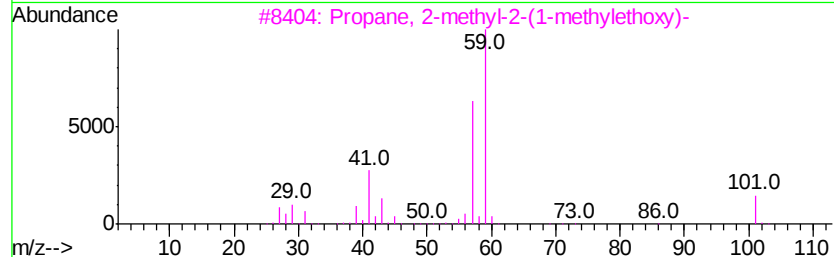
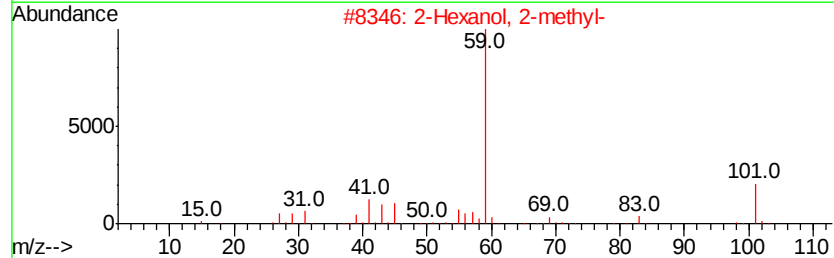
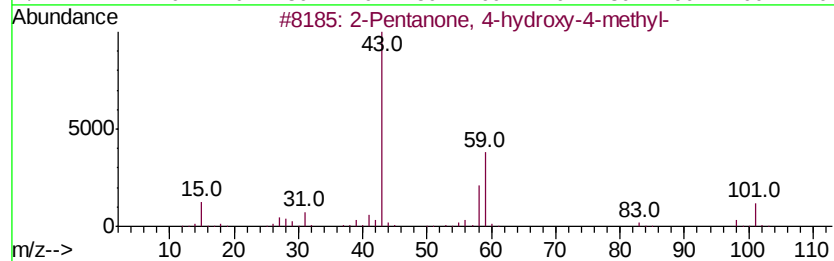
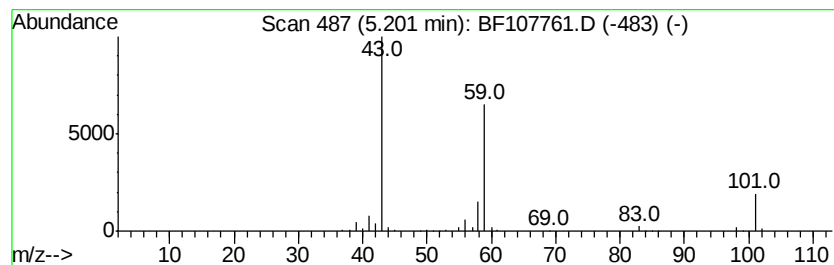
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.20	12.81 ng	597743	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	56
2			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
3			Propane, 2-methyl-2-(1-methylethoxy)-	116	C7H16O	017348-59-3	28
4			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
5			Acetic acid, cyano-, 1,1-dimethyl-	141	C7H11NO2	001116-98-9	23



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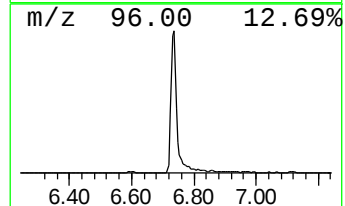
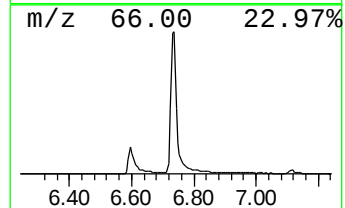
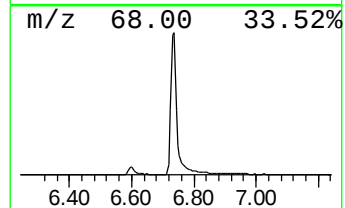
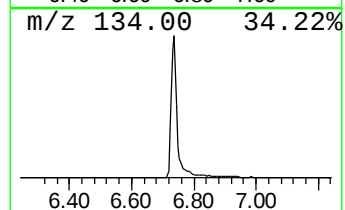
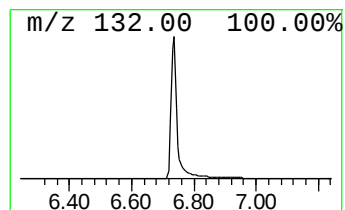
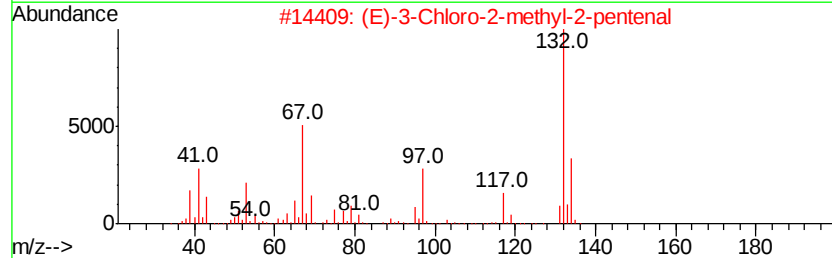
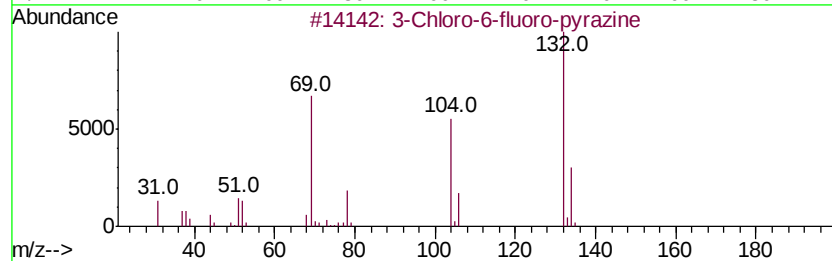
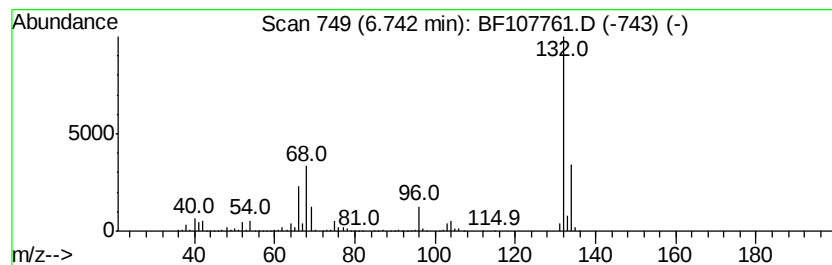
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Peak Number 2 unknown6.74 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	82.70 ng	3858740	1,4-Dichlorobenzene-d4	6.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	9



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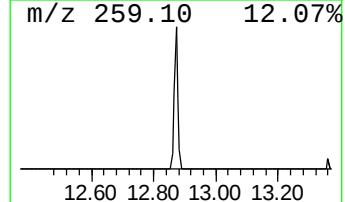
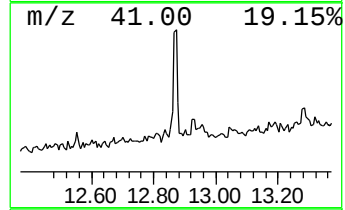
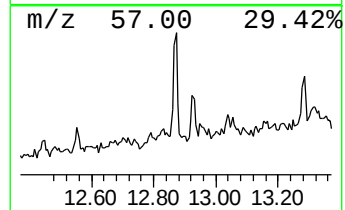
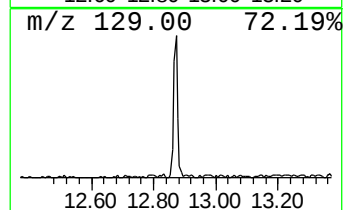
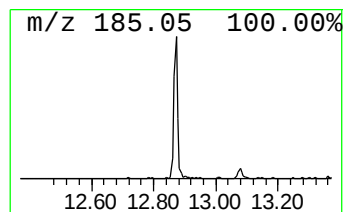
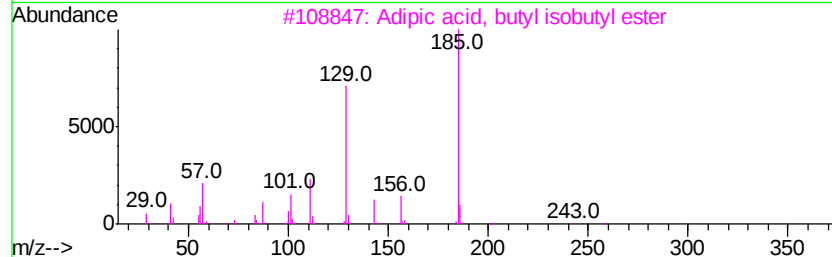
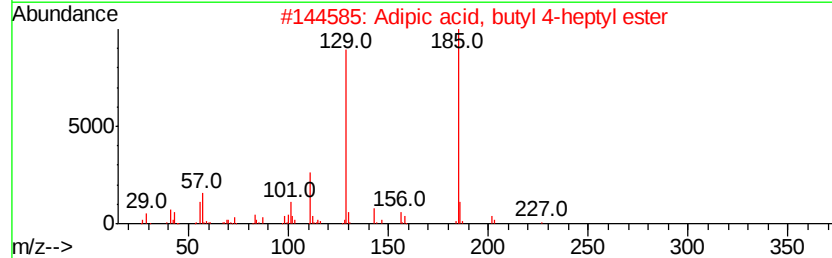
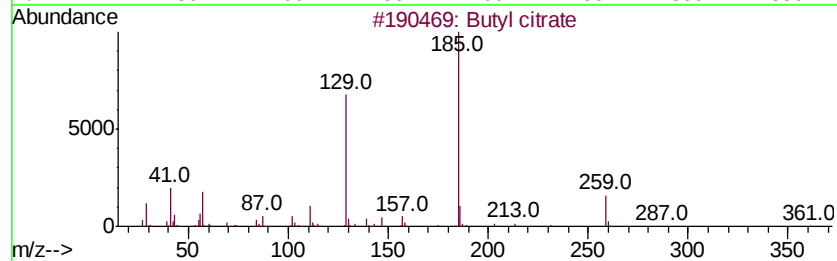
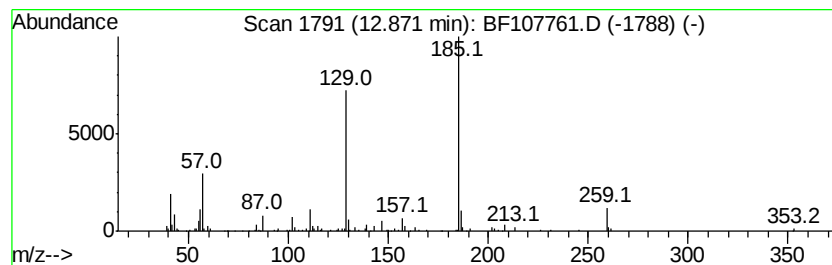
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Peak Number 4 Butyl citrate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.87	2.05 ng	130297	Chrysene-d12	14.15
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Butyl citrate	360 C18H32O7	000077-94-1	90
2	Adipic acid, butyl 4-heptyl ester	300 C17H32O4	1000349-73-7	64
3	Adipic acid, butyl isobutyl ester	258 C14H26O4	1000324-09-3	64
4	Adipic acid, 2-heptyl isobutyl e...	300 C17H32O4	1000353-64-3	56
5	Adipic acid, 2,4-dimethylpent-3-...	300 C17H32O4	1000349-77-6	56



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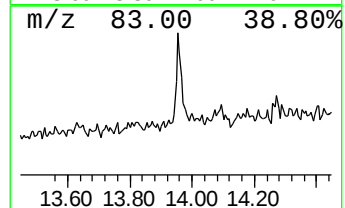
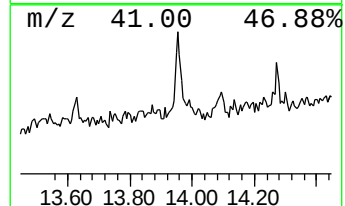
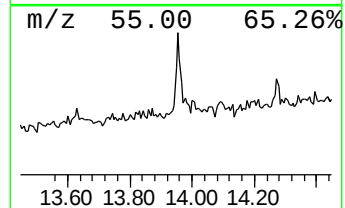
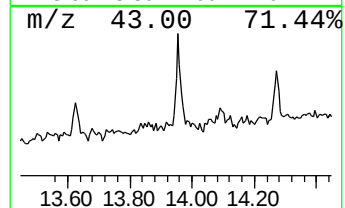
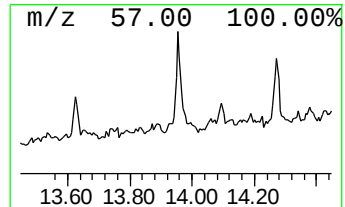
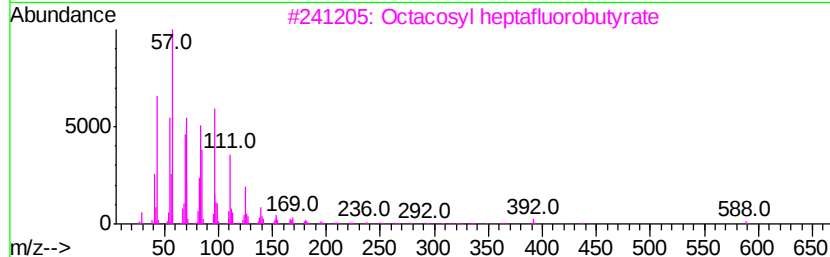
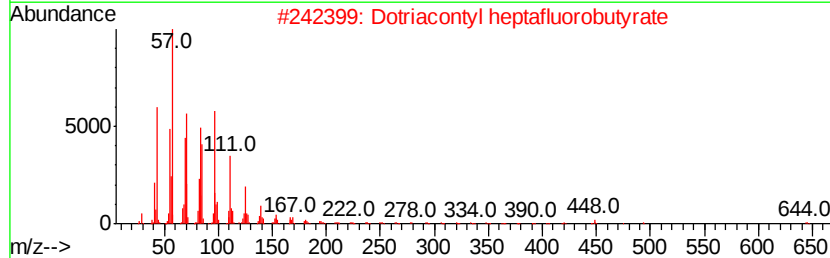
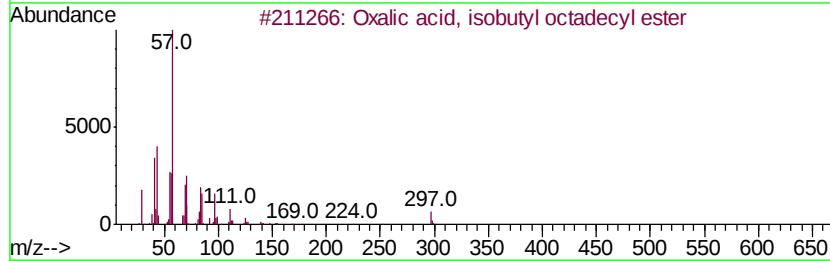
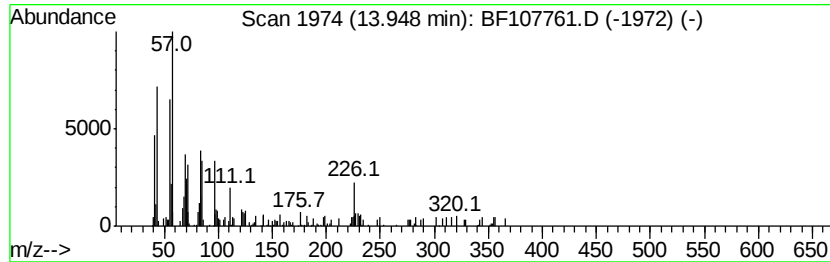
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Peak Number 6 Oxalic acid, isobutyl octadecyl... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.		
13.95	2.31 ng	147045	Chrysene-d12	14.15		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxalic acid, isobutyl octadecyl ...	398	C24H46O4	1000309-38-3	91	
2	Dotriacontyl heptafluorobutyrate	662	C36H65F7O2	1000351-84-2	91	
3	Octacosyl heptafluorobutyrate	606	C32H57F7O2	1000351-83-6	91	
4	Oxalic acid, cyclobutyl hexadecyl...	368	C22H40O4	1000309-70-6	91	
5	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	91	



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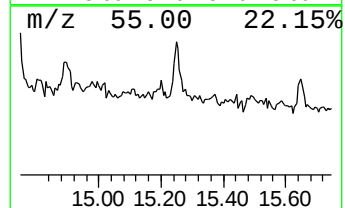
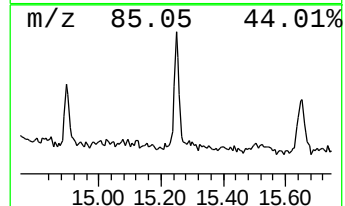
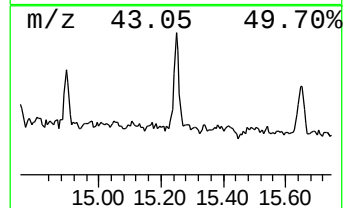
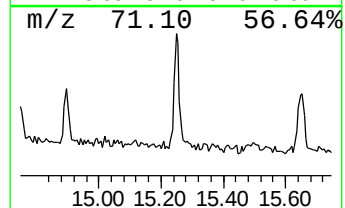
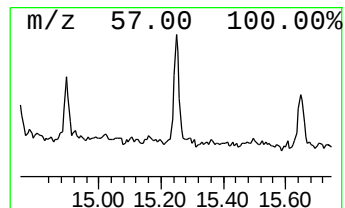
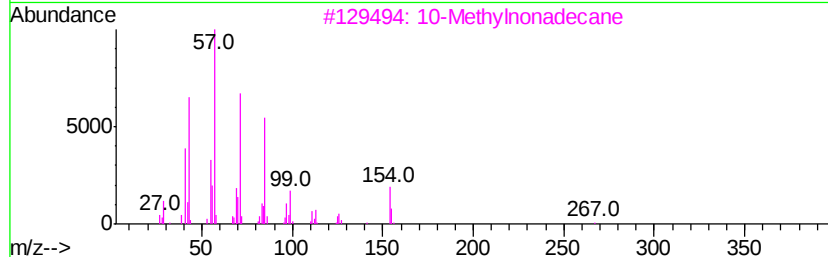
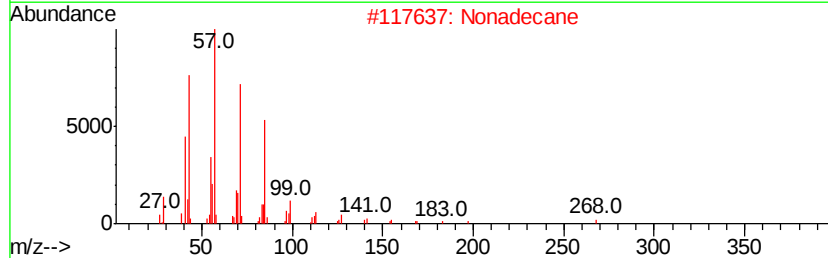
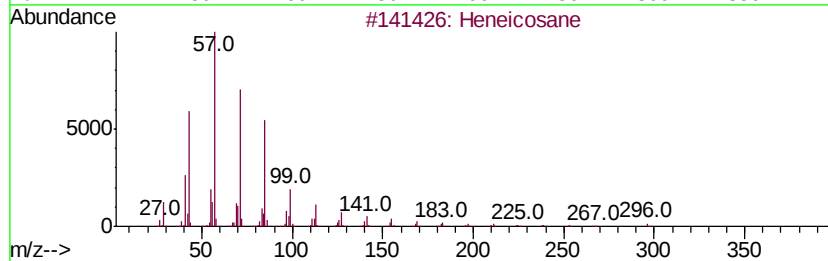
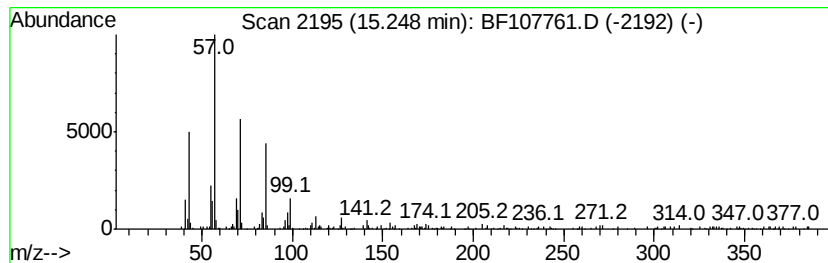
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Heneicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.25	3.68 ng	184429	Perylene-d12	15.68

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	93
2	Nonadecane		268	C19H40	000629-92-5	89
3	10-Methylnonadecane		282	C20H42	056862-62-5	83
4	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	80
5	Tridecane, 1-iodo-		310	C13H27I	035599-77-0	80



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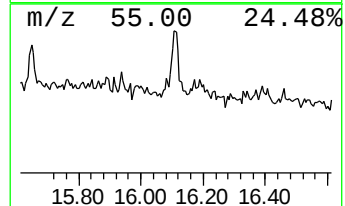
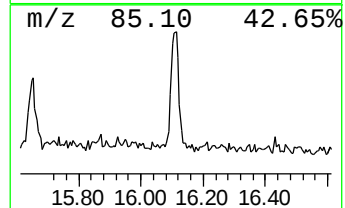
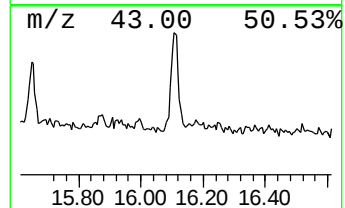
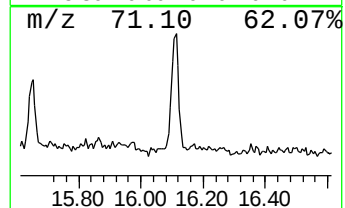
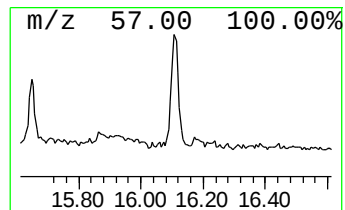
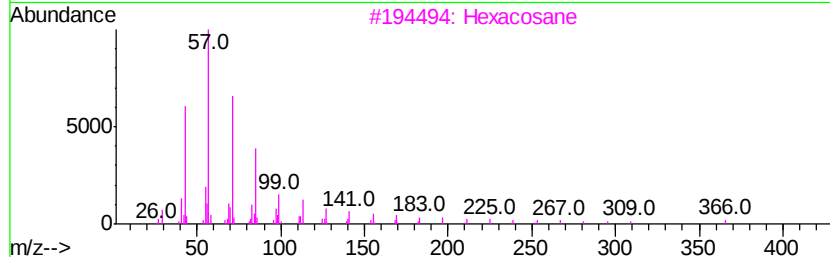
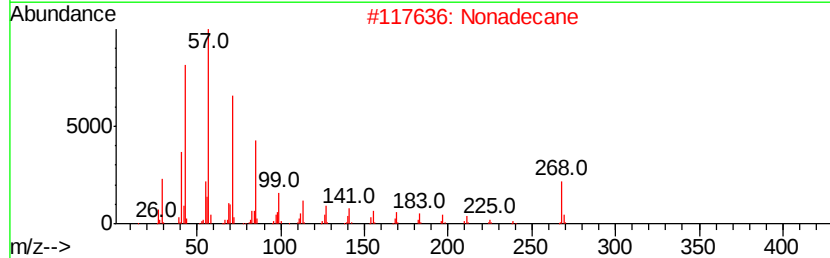
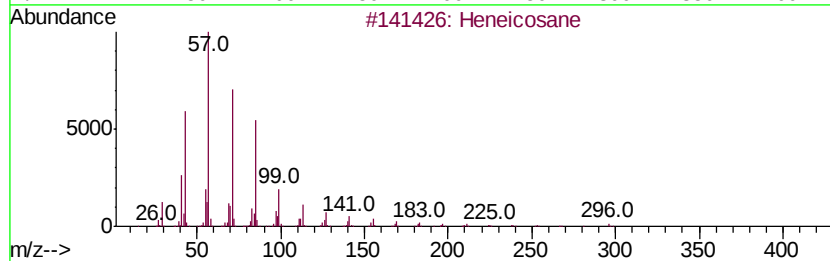
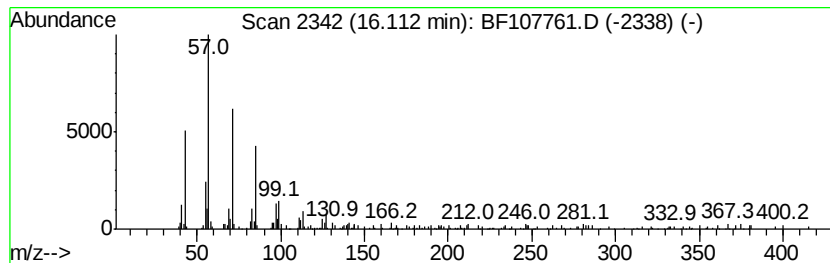
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Nonadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.11	3.63 ng	182021	Perylene-d12	15.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	90
2		Nonadecane	268	C19H40	000629-92-5	87
3		Hexacosane	366	C26H54	000630-01-3	87
4		Heptacosane	380	C27H56	000593-49-7	86
5		2-methyloctacosane	408	C29H60	1000376-72-8	80



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF072718\
Data File : BF107761.D
Acq On : 27 Jul 2018 22:10
Operator : JU/SJ
Sample : J4112-02
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CON-SB-08-09-0-11

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	12.8	ng	597743	1	6.96	933229	20.0
unknown6.74	6.74	82.7	ng	3858740	1	6.96	933229	20.0
Butyl citrate	12.87	2.0	ng	130297	5	14.15	1270730	20.0
Oxalic acid, isob...	13.95	2.3	ng	147045	5	14.15	1270730	20.0
Heneicosane	15.25	3.7	ng	184429	6	15.68	1003280	20.0
Nonadecane	16.11	3.6	ng	182021	6	15.68	1003280	20.0