

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF031219\
 Data File : BF113008.D
 Acq On : 12 Mar 2019 17:42
 Operator : JU/SJ
 Sample : K1697-01 5X
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SU-03-031119-A

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-BF022719.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	5.334	549	552	566	rBV	516076	572110	39.36%	4.356%
2	6.363	723	727	739	rBV	622677	619268	42.61%	4.715%
3	6.498	746	750	758	rBV	788506	654750	45.05%	4.985%
4	6.734	786	790	800	rBV	1120025	1000428	68.83%	7.617%
5	6.887	812	816	826	rBV	609920	522876	35.98%	3.981%
6	7.287	880	884	897	rBV	306569	354457	24.39%	2.699%
7	8.016	1004	1008	1015	rBV	1025426	1156947	79.60%	8.809%
8	9.086	1187	1190	1204	rBV	592399	729509	50.19%	5.555%
9	9.180	1204	1206	1214	rVB3	14232	19819	1.36%	0.151%
10	9.480	1255	1257	1263	rBV	29857	37199	2.56%	0.283%
11	9.763	1301	1305	1319	rBV	1240468	1292227	88.91%	9.839%
12	10.545	1435	1438	1453	rBV	331231	398467	27.42%	3.034%
13	10.675	1458	1460	1465	rBV	13073	16502	1.14%	0.126%
14	11.122	1533	1536	1541	rBV3	11597	17113	1.18%	0.130%
15	11.239	1552	1556	1567	rBV	1109306	1210389	83.28%	9.216%
16	11.316	1567	1569	1574	rVB	13478	18051	1.24%	0.137%
17	11.645	1622	1625	1631	rVB	51300	44870	3.09%	0.342%
18	11.774	1644	1647	1658	rBV3	62631	93704	6.45%	0.713%
19	12.321	1737	1740	1742	rBV	162352	148466	10.21%	1.130%
20	12.345	1742	1744	1751	rVB2	244512	224884	15.47%	1.712%
21	12.445	1756	1761	1765	rBV2	38513	55769	3.84%	0.425%
22	12.563	1778	1781	1785	rBV4	24382	34425	2.37%	0.262%
23	12.674	1794	1800	1803	rBV	37410	45824	3.15%	0.349%
24	12.816	1820	1824	1833	rBV	661957	659316	45.36%	5.020%
25	13.004	1850	1856	1861	rBV4	11612	20726	1.43%	0.158%
26	13.068	1863	1867	1871	rVB6	13578	19233	1.32%	0.146%
27	13.727	1976	1979	1986	rBV3	36939	55624	3.83%	0.424%
28	13.863	1998	2002	2015	rBV	1238069	1453431	100.00%	11.067%
29	14.045	2030	2033	2038	rVB	35922	32409	2.23%	0.247%
30	14.345	2081	2084	2087	rBV	66545	58149	4.00%	0.443%
31	14.645	2132	2135	2138	rBV	88868	88542	6.09%	0.674%
32	14.957	2185	2188	2192	rVB	103471	113585	7.81%	0.865%
33	15.268	2237	2241	2246	rBV	806651	1093901	75.26%	8.329%
34	15.310	2246	2248	2257	rVB	116927	159674	10.99%	1.216%

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ClientSampleId :
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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-BF022719.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.721	2314	2318	2323	rBV	73264	110671	7.61%	0.843%
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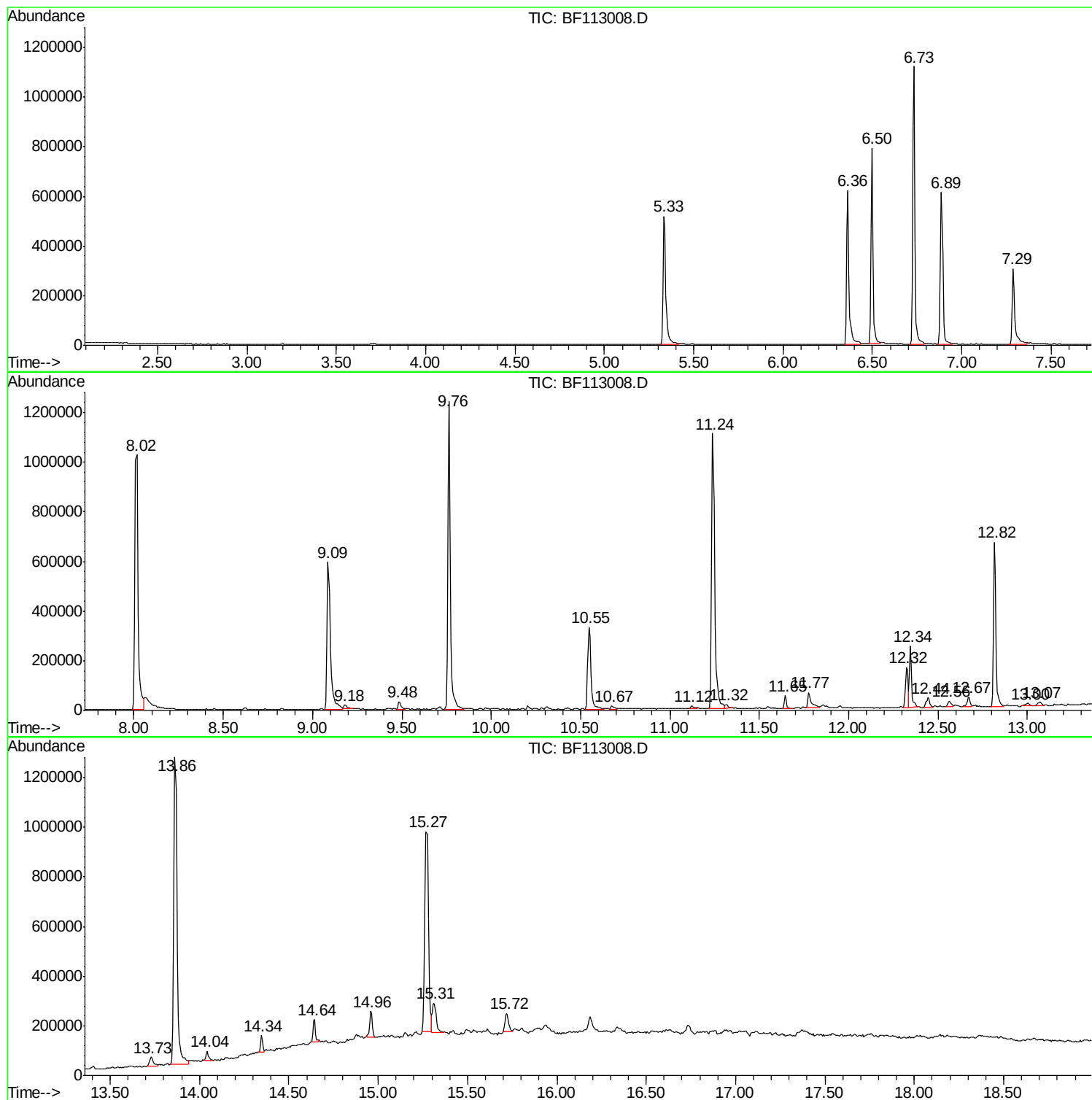
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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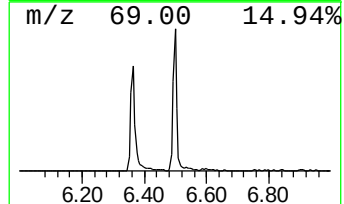
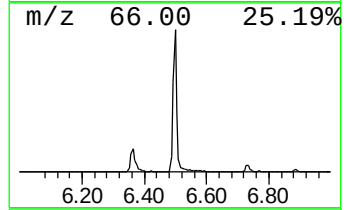
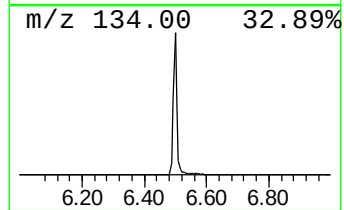
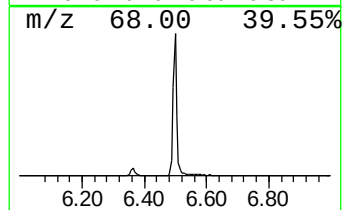
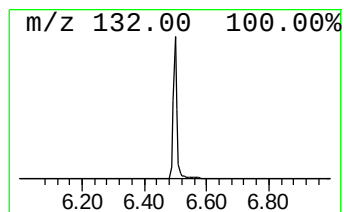
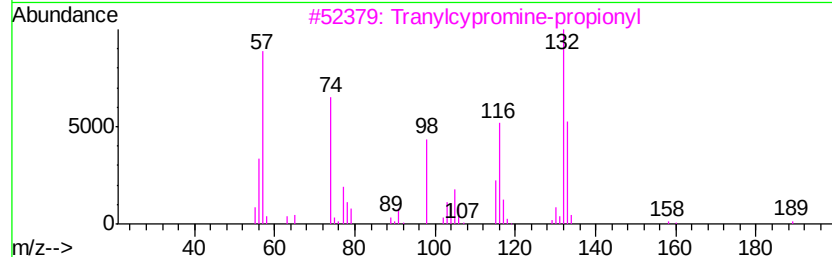
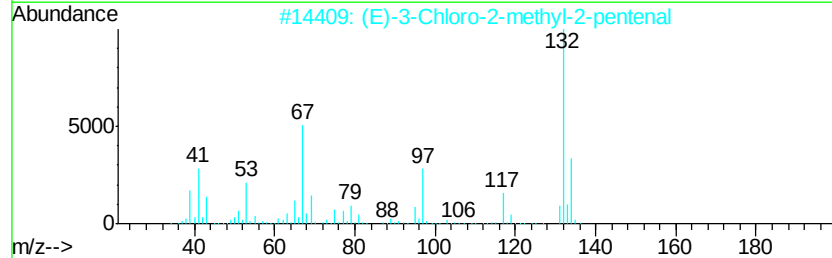
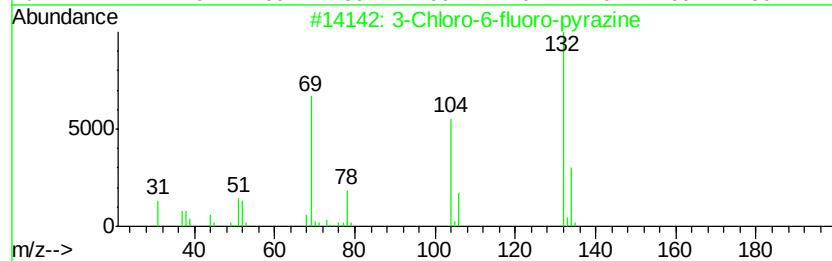
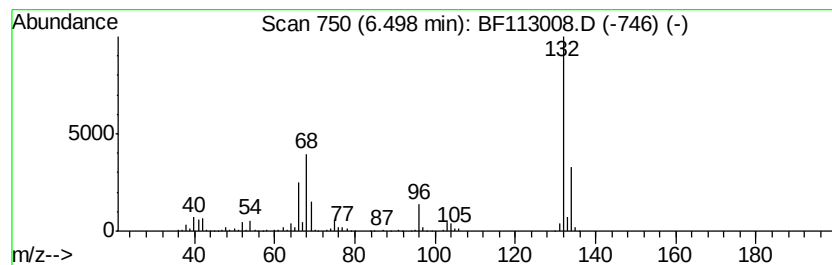
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	13.09 ng	654750	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		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		5-Aminoindole	132	C8H8N2	005192-03-0	12
5		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



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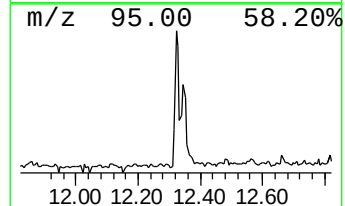
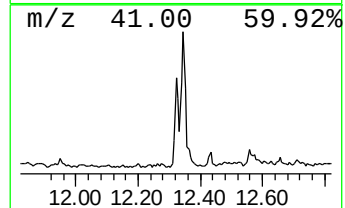
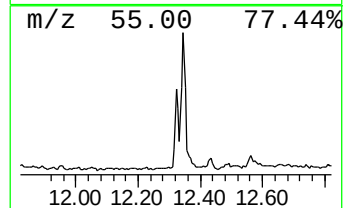
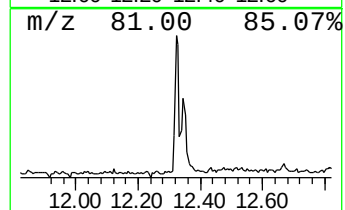
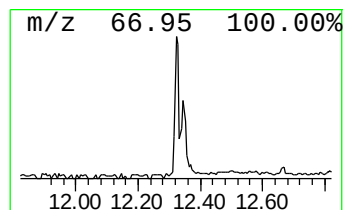
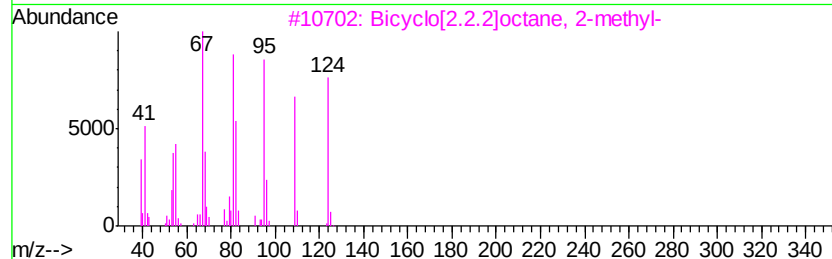
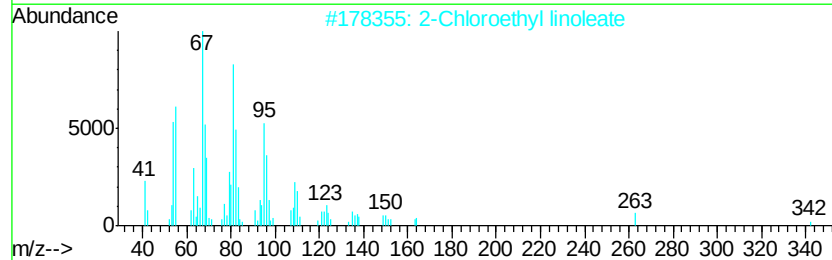
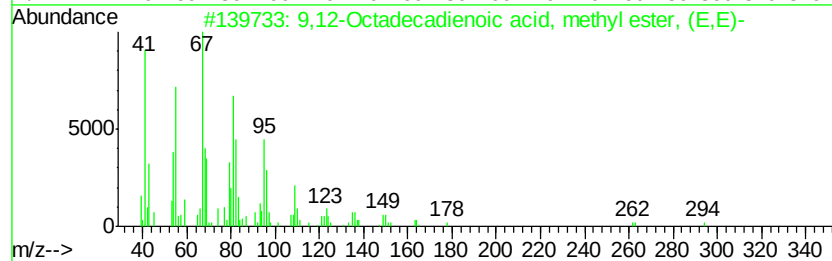
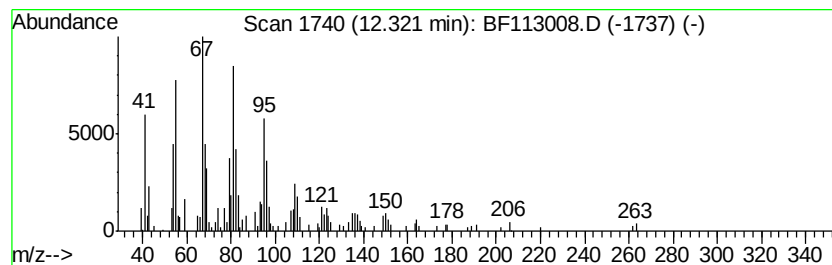
Instrument :
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 9,12-Octadecadienoic acid, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.		
12.32	2.45 ng	148466	Phenanthrene-d10	11.24		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	93	
2	2-Chloroethyl linoleate	342	C20H35ClO2	025525-76-2	91	
3	Bicyclo[2.2.2]octane, 2-methyl-	124	C9H16	000766-53-0	91	
4	7-Hexadecyne	222	C16H30	074685-28-2	83	
5	11,14-Eicosadienoic acid, methyl...	322	C21H38O2	002463-02-7	76	



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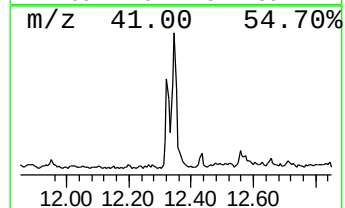
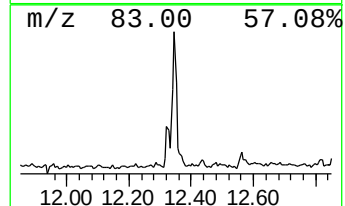
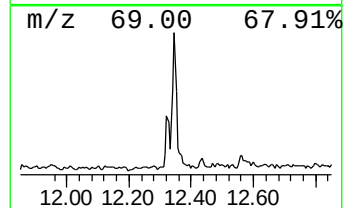
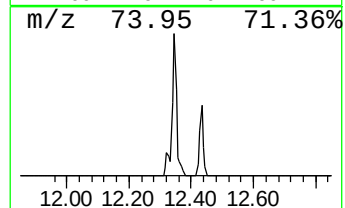
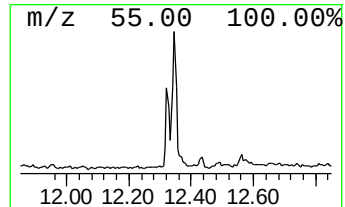
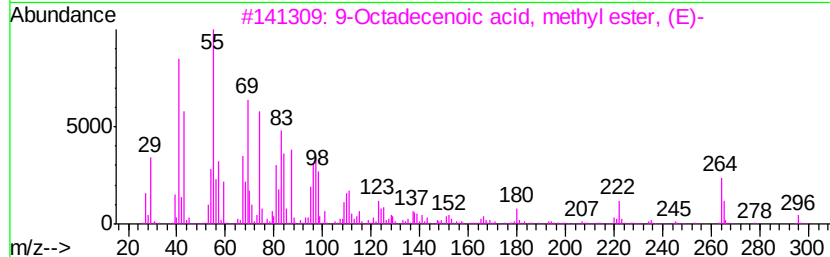
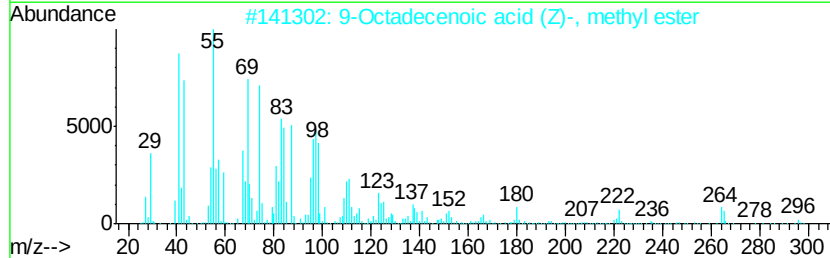
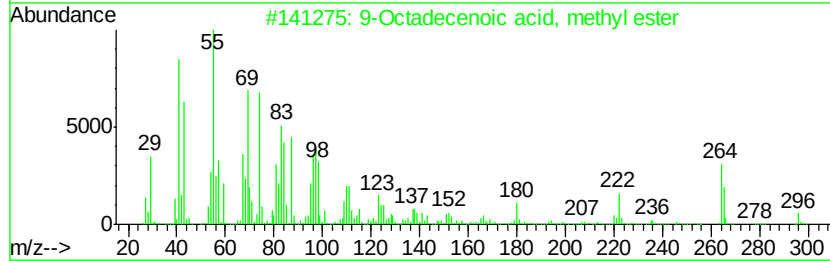
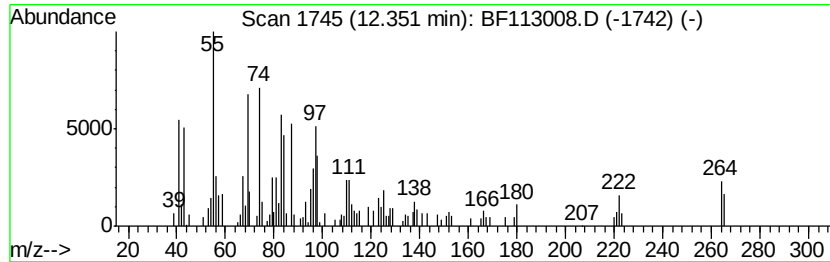
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 9-Octadecenoic acid, methyl... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.35	3.72 ng	224884	Phenanthrene-d10	11.24	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid, methyl ester	296	C19H36O2	002462-84-2	99
2	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	99
3	9-Octadecenoic acid, methyl este...	296	C19H36O2	001937-62-8	99
4	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	99
5	11-Octadecenoic acid, methyl est...	296	C19H36O2	001937-63-9	98



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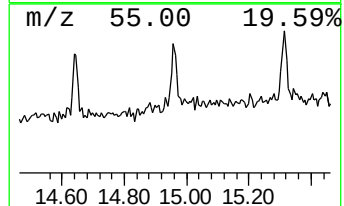
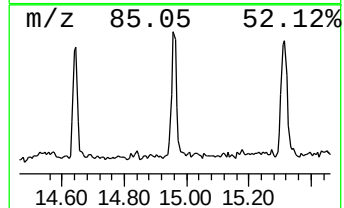
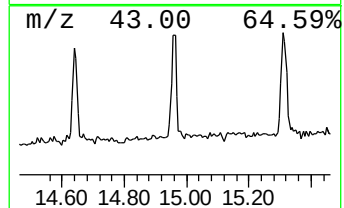
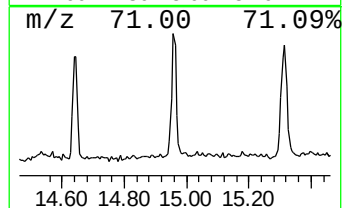
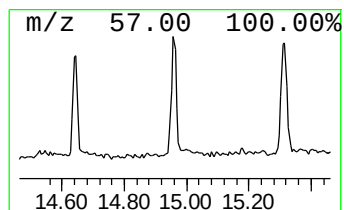
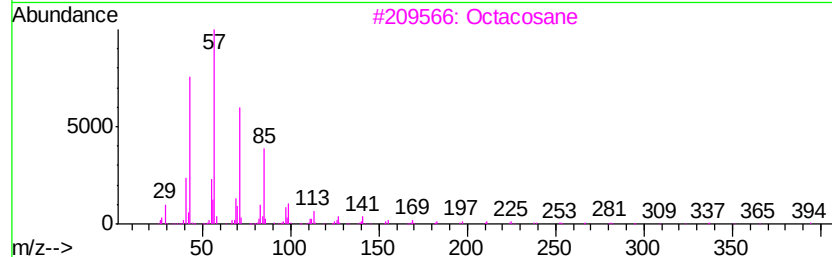
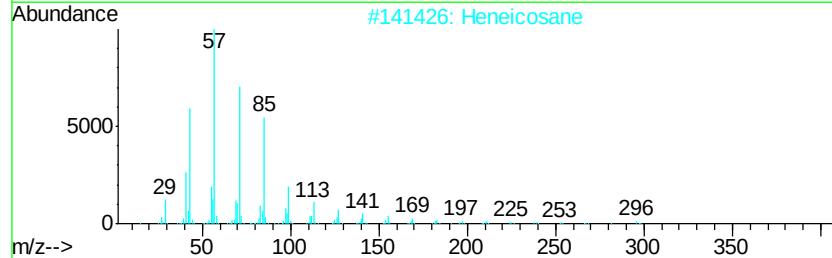
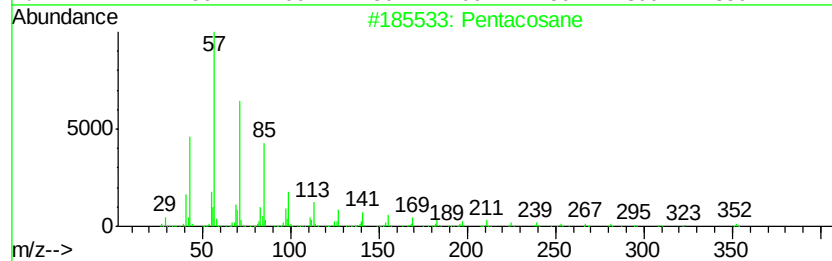
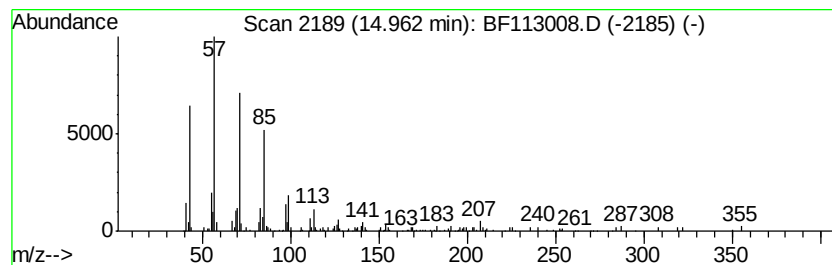
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 5 Pentacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.96	2.08 ng	113585	Perylene-d12	15.27

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane		352	C25H52	000629-99-2	94
2	Heneicosane		296	C21H44	000629-94-7	87
3	Octacosane		394	C28H58	000630-02-4	86
4	Eicosane		282	C20H42	000112-95-8	86
5	Docosane		310	C22H46	000629-97-0	86



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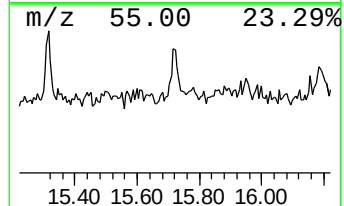
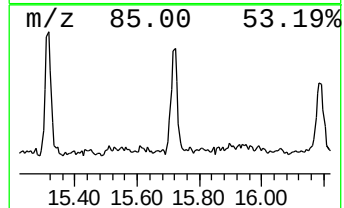
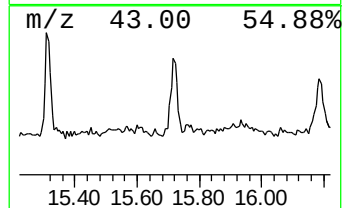
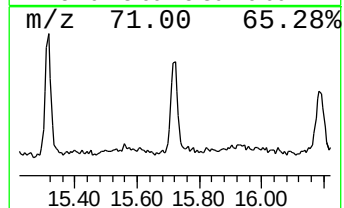
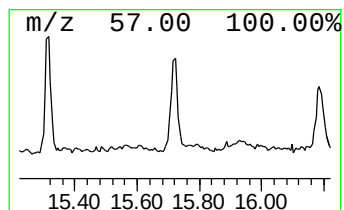
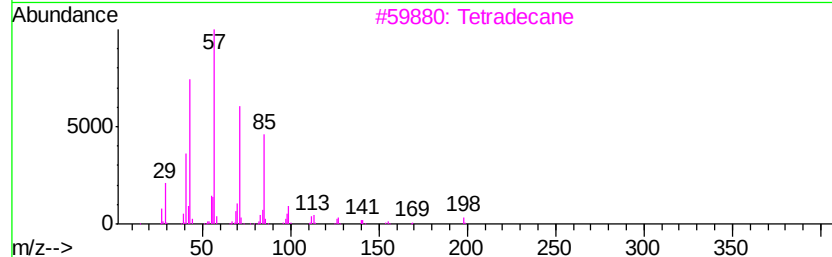
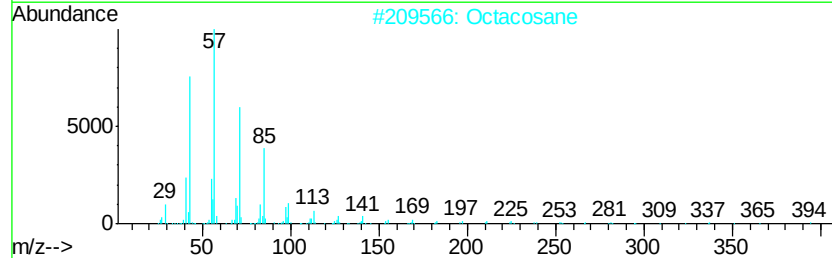
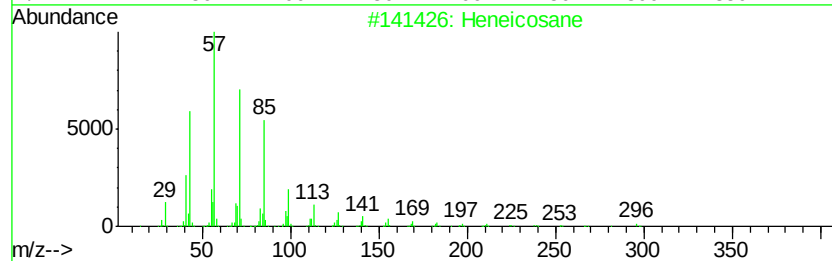
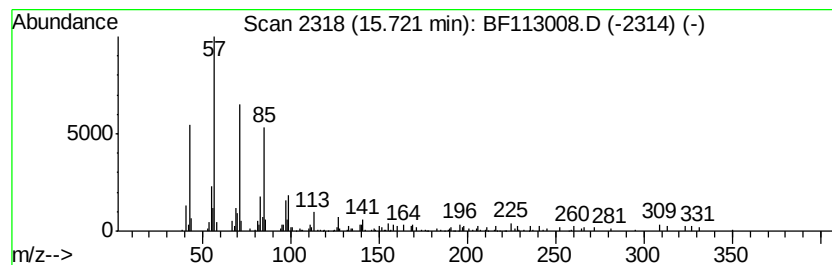
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.72	2.02 ng	110671	Perylene-d12	15.27

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	90
2	Octacosane		394	C28H58	000630-02-4	90
3	Tetradecane		198	C14H30	000629-59-4	87
4	triacontane		422	C30H62	000638-68-6	87
5	Hexadecane, 1-iodo-		352	C16H33I	000544-77-4	87



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Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-03-031119-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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
unknown6.50	6.50	13.1	ng	654750	1	6.73	1000430	20.0
9,12-Octadecadien...	12.32	2.5	ng	148466	4	11.24	1210390	20.0
9-Octadecenoic ac...	12.35	3.7	ng	224884	4	11.24	1210390	20.0
Pentacosane	14.96	2.1	ng	113585	6	15.27	1093900	20.0
Heneicosane	15.72	2.0	ng	110671	6	15.27	1093900	20.0