

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF090518\
 Data File : BF108815.D
 Acq On : 6 Sep 2018 10:18
 Operator : JU/SJ
 Sample : J4724-09
 Misc :
 ALS Vial : 33 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 EP1-SUT-UST-08

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	4.931	437	441	452	rVB	124116	161458	3.82%	0.386%
2	5.348	507	512	515	rBV	3800264	3618417	85.65%	8.657%
3	6.366	680	685	688	rBV	3881531	3866498	91.52%	9.250%
4	6.501	704	708	712	rBV	4025576	3829312	90.64%	9.161%
5	6.566	716	719	729	rVB	121045	113789	2.69%	0.272%
6	6.736	744	748	751	rBV	2091331	1626310	38.49%	3.891%
7	6.895	771	775	778	rBV	3256421	3041874	72.00%	7.277%
8	7.295	838	843	846	rBV	2589589	2361797	55.90%	5.650%
9	8.019	962	966	969	rBV	2273980	1997678	47.28%	4.779%
10	9.095	1144	1149	1152	rBV	4584671	4224767	100.00%	10.107%
11	9.219	1167	1170	1173	rVB	53768	45888	1.09%	0.110%
12	9.483	1211	1215	1218	rBV	1626254	1296335	30.68%	3.101%
13	9.766	1259	1263	1267	rBV	2443811	1998474	47.30%	4.781%
14	10.548	1392	1396	1399	rBV	2247691	1961358	46.43%	4.692%
15	10.701	1416	1422	1426	rVB	58607	72591	1.72%	0.174%
16	11.160	1497	1500	1506	rVB	60933	65660	1.55%	0.157%
17	11.242	1510	1514	1516	rVV	2082904	1695685	40.14%	4.057%
18	11.266	1516	1518	1521	rVV	190183	153562	3.63%	0.367%
19	11.313	1522	1526	1529	rVB	62329	64362	1.52%	0.154%
20	11.783	1601	1606	1610	rBV2	193657	231745	5.49%	0.554%
21	12.448	1716	1719	1723	rBV	339329	296617	7.02%	0.710%
22	12.565	1736	1739	1743	rBV5	35328	51926	1.23%	0.124%
23	12.671	1752	1757	1760	rBV	354299	345865	8.19%	0.827%
24	12.824	1779	1783	1786	rBV	3573444	3093504	73.22%	7.401%
25	13.101	1828	1830	1833	rBV2	44369	49226	1.17%	0.118%
26	13.412	1881	1883	1886	rVB	57306	45616	1.08%	0.109%
27	13.501	1896	1898	1902	rBV	41436	45588	1.08%	0.109%
28	13.730	1934	1937	1945	rVB	460539	493433	11.68%	1.181%
29	13.865	1956	1960	1963	rBV	2018567	1864657	44.14%	4.461%
30	13.889	1963	1964	1967	rVB	143073	88489	2.09%	0.212%
31	14.054	1990	1992	1995	rVB2	82978	73346	1.74%	0.175%
32	14.359	2041	2044	2049	rBV	132475	163553	3.87%	0.391%
33	14.659	2092	2095	2100	rVB	119757	125010	2.96%	0.299%
34	14.724	2104	2106	2110	rVB	191667	186376	4.41%	0.446%

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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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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.871	2128	2131	2134	rBV	131309	177798	4.21%	0.425%
36	14.977	2146	2149	2155	rVB	156041	166550	3.94%	0.398%
37	15.154	2177	2179	2184	rVB	99184	115130	2.73%	0.275%
38	15.212	2186	2189	2194	rVV	123524	166058	3.93%	0.397%
39	15.271	2195	2199	2204	rVV	1227605	1551288	36.72%	3.711%
40	15.330	2207	2209	2215	rVB	135402	158620	3.75%	0.379%
41	15.742	2276	2279	2283	rBV2	92199	112302	2.66%	0.269%

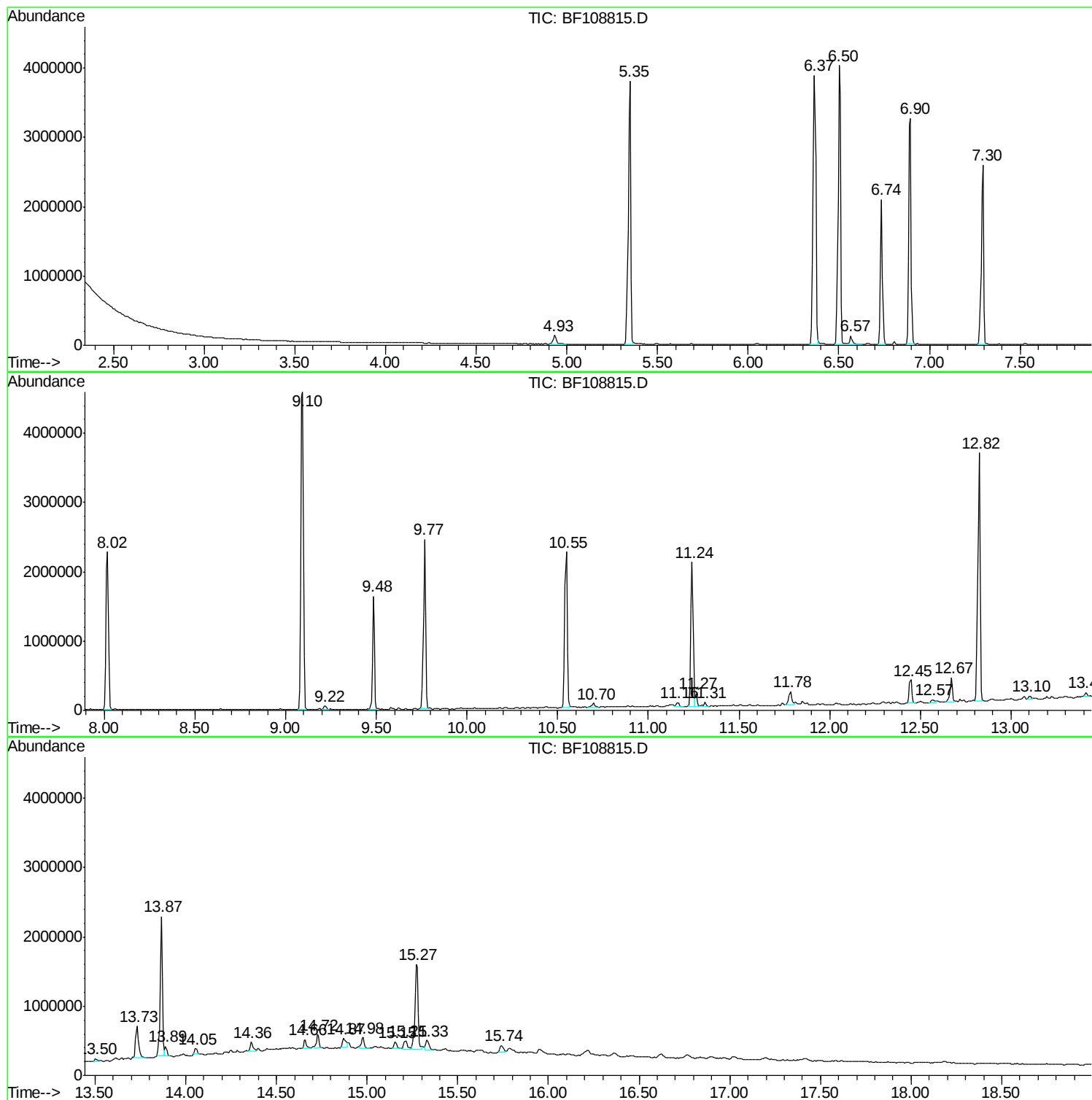
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF090518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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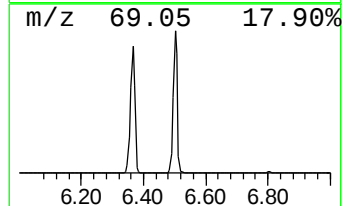
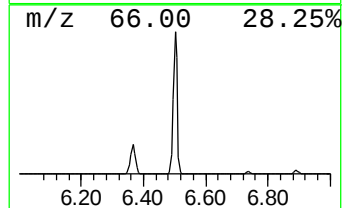
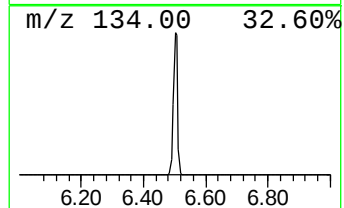
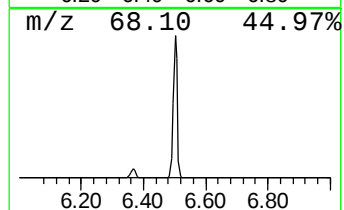
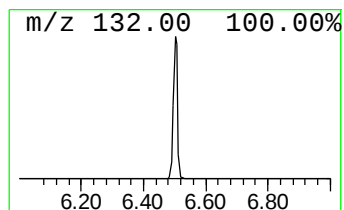
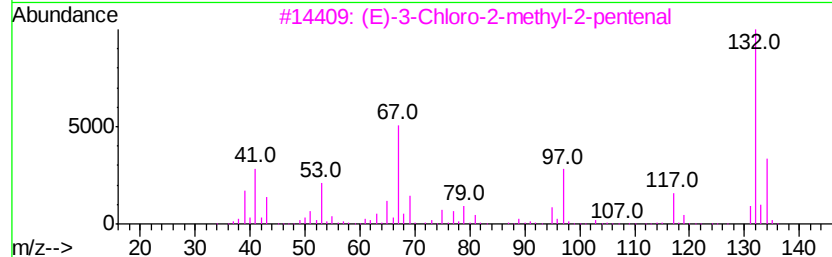
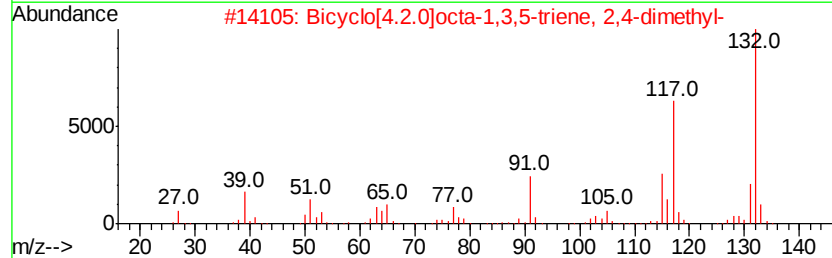
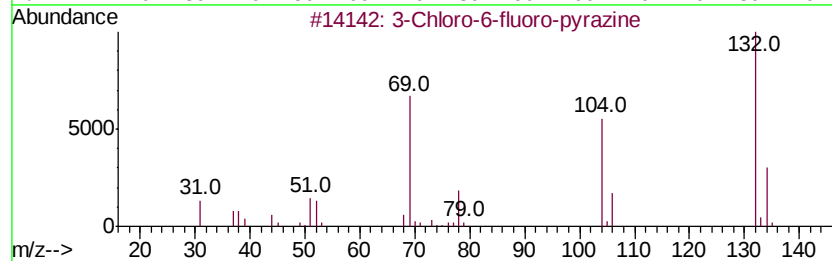
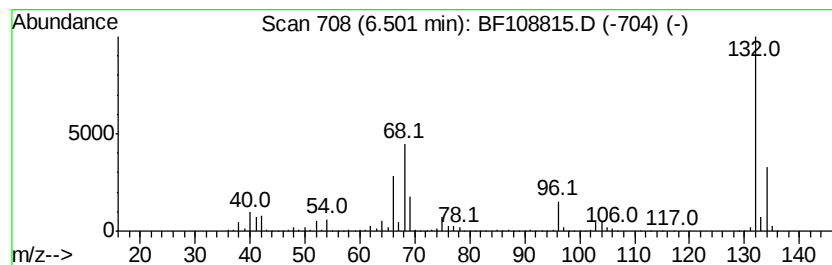
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	47.09 ng	3829310	1,4-Dichlorobenzene-d4	6.74

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	Bicyclo[4.2.0]octa-1,3,5-triene, ...			132	C10H12	028749-81-7	9
3	(E)-3-Chloro-2-methyl-2-pentenal			132	C6H9ClO	031357-76-3	9
4	4-Chloro-2-fluoro-pyrimidine			132	C4H2ClFN2	051422-00-5	9
5	1-Methylpyrrolo[1,2-a]pyrazine			132	C8H8N2	064608-59-9	9



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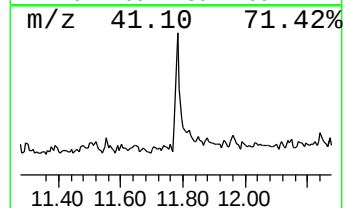
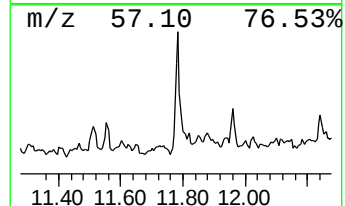
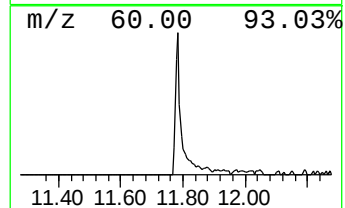
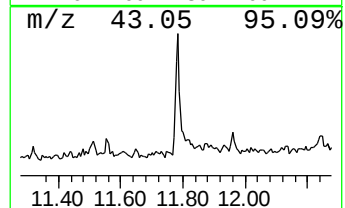
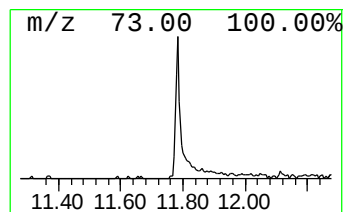
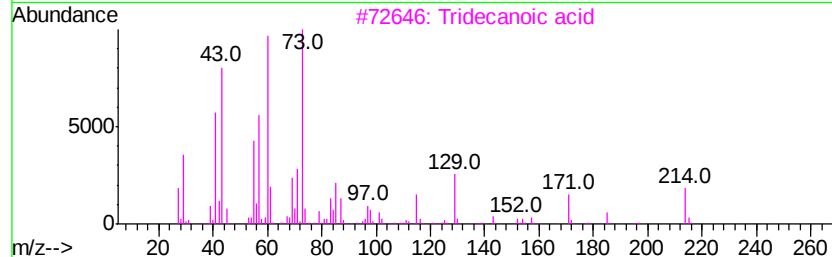
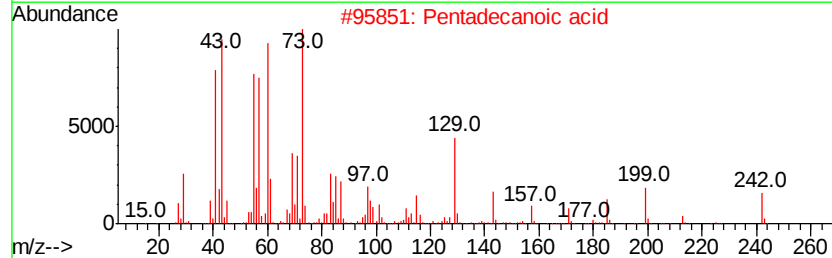
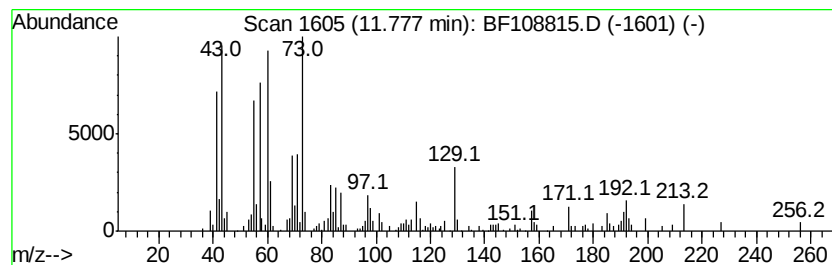
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.78	2.73 ng	231745	Phenanthrene-d10	11.24

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3		Tridecanoic acid	214	C13H26O2	000638-53-9	89
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	86
5		n-Decanoic acid	172	C10H20O2	000334-48-5	76



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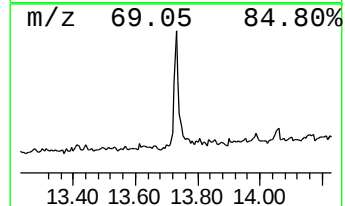
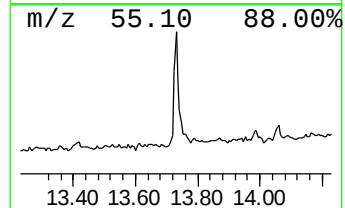
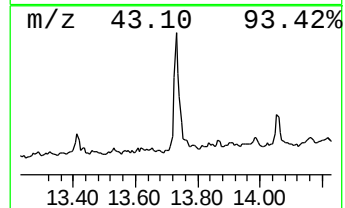
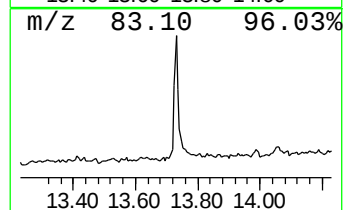
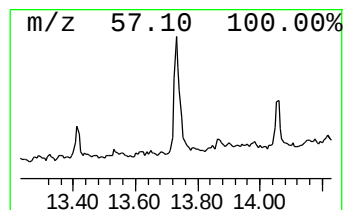
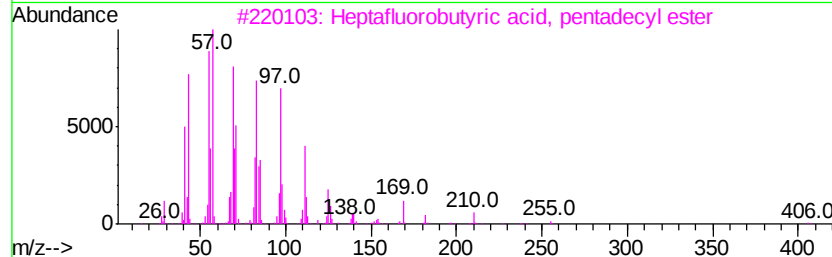
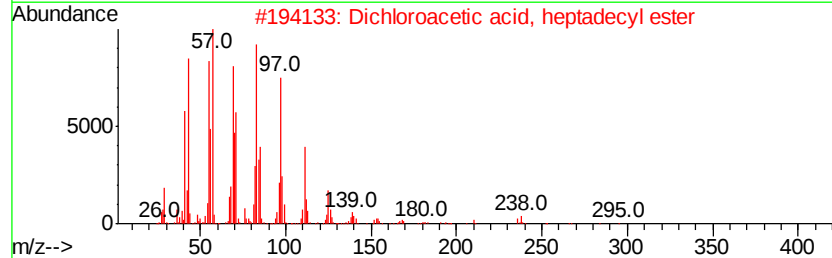
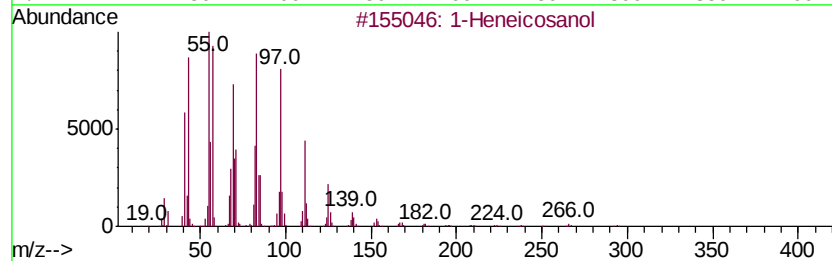
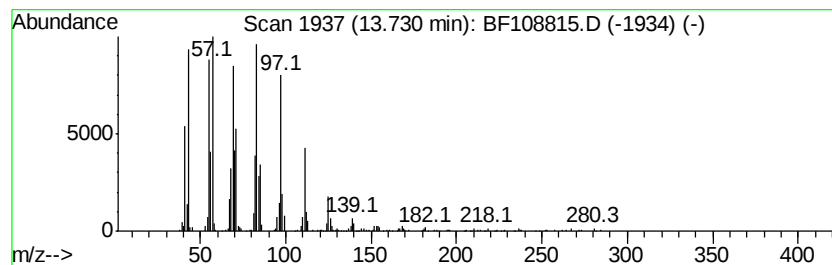
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.73	5.29 ng	493433	Chrysene-d12	13.87
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Heneicosanol	312 C21H44O	015594-90-8	95
2	Dichloroacetic acid, heptadecyl ...	366 C19H36Cl2O2	1000282-98-2	94
3	Heptafluorobutyric acid, pentade...	424 C19H31F7O2	959261-23-5	94
4	Trifluoroacetic acid, pentadecyl...	324 C17H31F3O2	959010-23-2	94
5	1-Heptacosanol	396 C27H56O	002004-39-9	94



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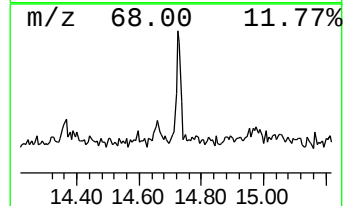
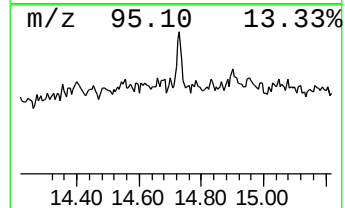
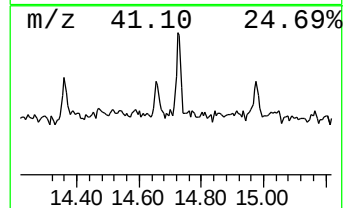
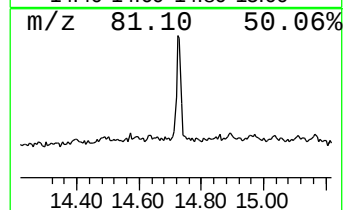
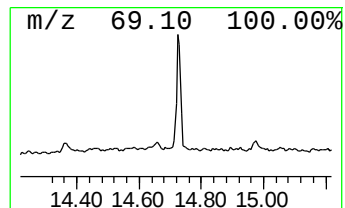
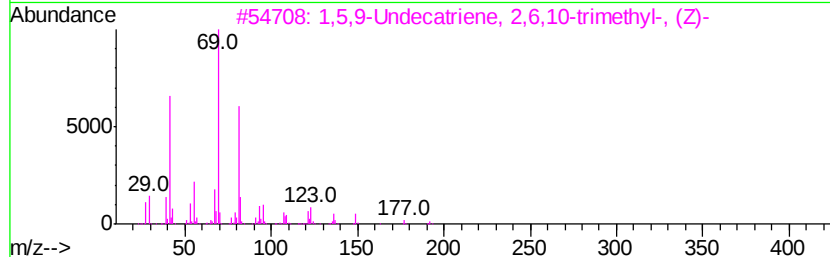
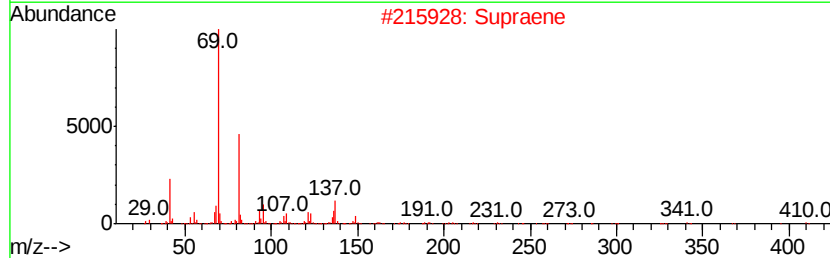
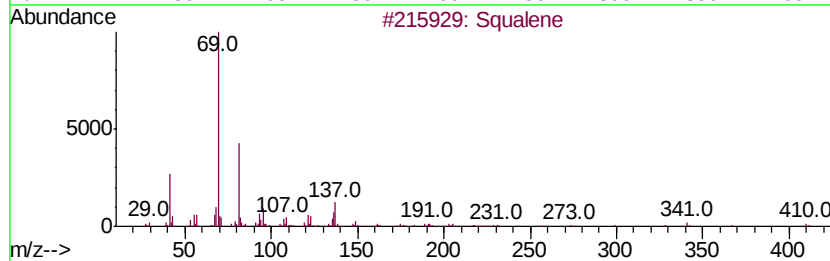
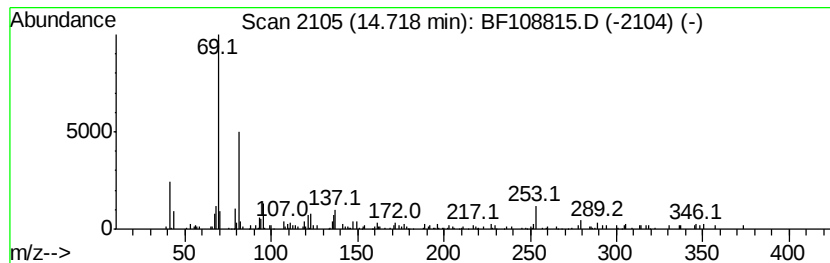
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.72	2.40 ng	186376	Perylene-d12	15.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	83
2		Supraene	410	C30H50	007683-64-9	83
3		1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	74
4		(E)-all-trans-3,7,11-Trimethyl-2...	235	C15H25NO	1000161-30-7	64
5		4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	64



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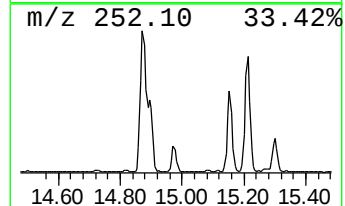
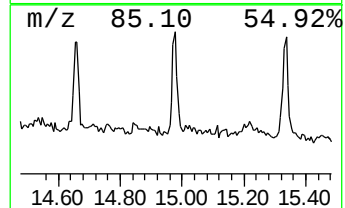
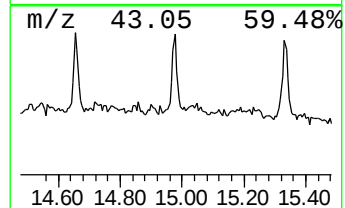
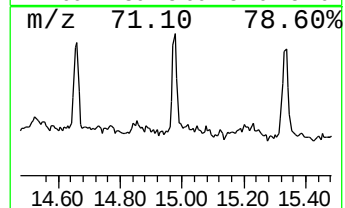
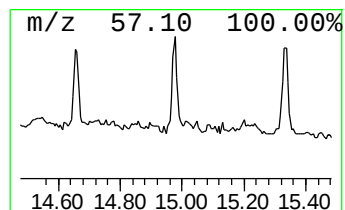
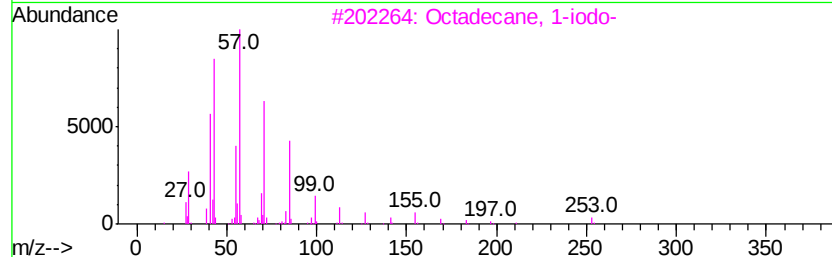
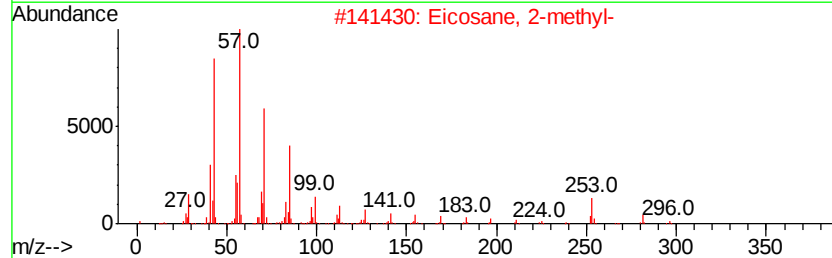
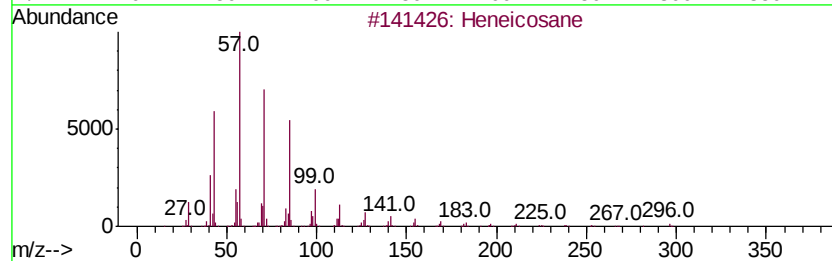
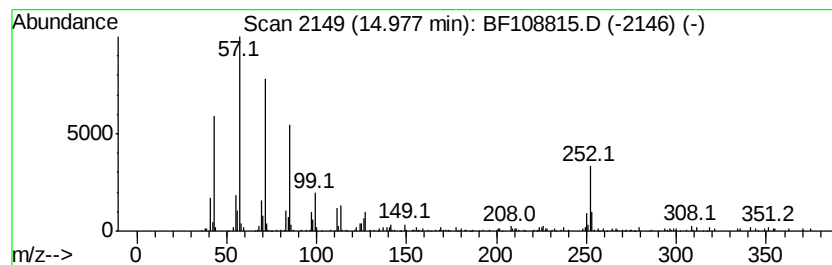
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Eicosane, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.		
14.98	2.15 ng	166550	Perylene-d12	15.28		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heneicosane	296	C21H44	000629-94-7	89
2		Eicosane, 2-methyl-	296	C21H44	001560-84-5	81
3		Octadecane, 1-iodo-	380	C18H37I	000629-93-6	72
4		Triacontane	422	C30H62	000638-68-6	72
5		Octacosane	394	C28H58	000630-02-4	68



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090518\
Data File : BF108815.D
Acq On : 6 Sep 2018 10:18
Operator : JU/SJ
Sample : J4724-09
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EP1-SUT-UST-08

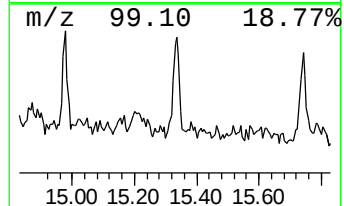
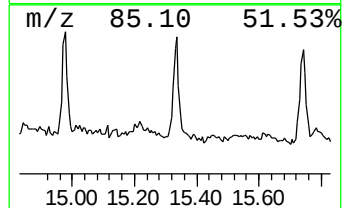
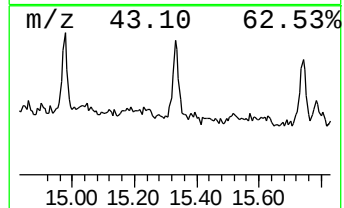
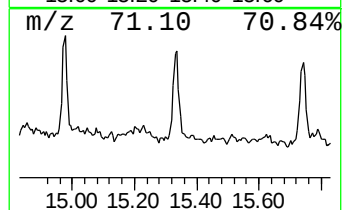
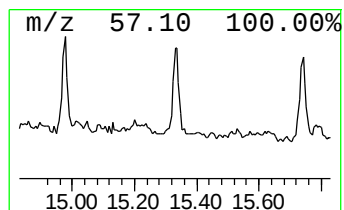
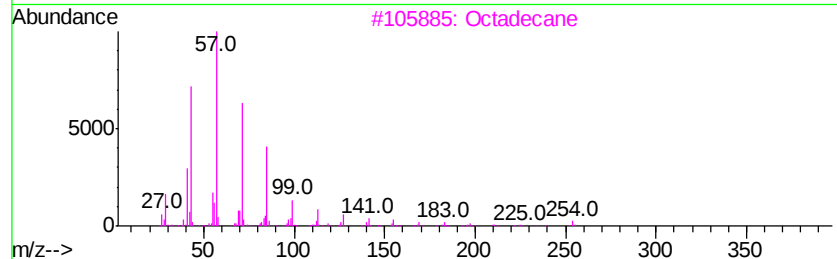
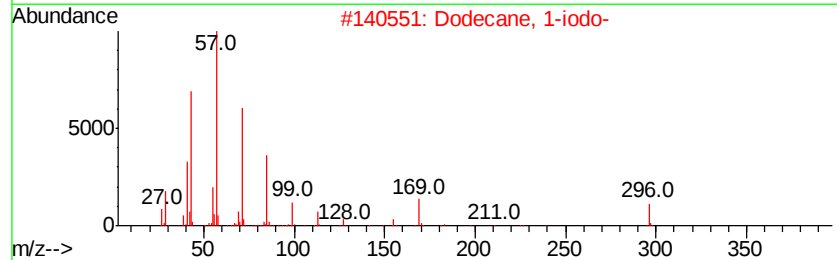
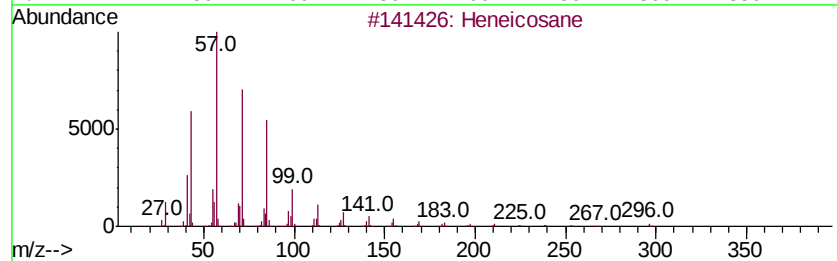
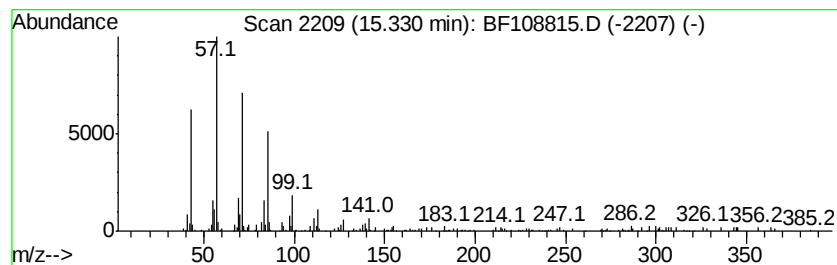
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
15.33	2.05 ng	158620	Perylene-d12	15.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	93
2		Dodecane, 1-iodo-	296	C12H25I	004292-19-7	90
3		Octadecane	254	C18H38	000593-45-3	90
4		Heptadecane	240	C17H36	000629-78-7	87
5		Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF090518\
Data File : BF108815.D
Acq On : 6 Sep 2018 10:18
Operator : JU/SJ
Sample : J4724-09
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EP1-SUT-UST-08

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
unknown6.50	6.50	47.1	ng	3829310	1	6.74	1626310	20.0
n-Hexadecanoic acid	11.78	2.7	ng	231745	4	11.24	1695690	20.0
1-Heneicosanol	13.73	5.3	ng	493433	5	13.87	1864660	20.0
Squalene	14.72	2.4	ng	186376	6	15.28	1551290	20.0
Eicosane, 2-methyl-	14.98	2.1	ng	166550	6	15.28	1551290	20.0
Heneicosane	15.33	2.0	ng	158620	6	15.28	1551290	20.0