

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF121118\
 Data File : BF111291.D
 Acq On : 11 Dec 2018 22:18
 Operator : JU/SJ
 Sample : J6157-09
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMPOSITE-5-TOTAL

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-BF120818.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	2.169	12	14	23	rVB	30236	52279	2.50%	0.242%
2	3.775	282	287	291	rBV2	29947	45216	2.16%	0.209%
3	4.022	324	329	334	rBV	48490	68902	3.30%	0.319%
4	4.957	485	488	490	rBV	81167	88138	4.22%	0.408%
5	4.975	490	491	495	rVB	76246	70611	3.38%	0.327%
6	5.398	559	563	573	rBV	529326	476947	22.83%	2.206%
7	5.739	618	621	625	rBV	25278	24628	1.18%	0.114%
8	5.916	648	651	654	rVB	73052	55101	2.64%	0.255%
9	6.428	733	738	749	rBV2	664252	877913	42.03%	4.061%
10	6.557	757	760	766	rBV	885872	760207	36.39%	3.517%
11	6.792	797	800	804	rBV	1761780	1544151	73.92%	7.143%
12	6.857	808	811	816	rVB	35893	33725	1.61%	0.156%
13	6.951	823	827	830	rBV	1042176	858969	41.12%	3.974%
14	7.345	891	894	904	rBV	777632	711841	34.08%	3.293%
15	7.575	930	933	936	rVB	44290	37088	1.78%	0.172%
16	8.075	1014	1018	1022	rBV	2371902	2088887	100.00%	9.664%
17	8.386	1068	1071	1083	rBV	28144	37347	1.79%	0.173%
18	9.151	1197	1201	1207	rBV	1411775	1108646	53.07%	5.129%
19	9.545	1264	1268	1271	rBV	669203	495484	23.72%	2.292%
20	9.727	1295	1299	1305	rBV4	20072	32362	1.55%	0.150%
21	9.833	1313	1317	1321	rBV	2237266	1938030	92.78%	8.966%
22	10.033	1348	1351	1360	rVB2	43863	43017	2.06%	0.199%
23	10.616	1446	1450	1454	rBV	515911	488976	23.41%	2.262%
24	10.745	1470	1472	1478	rBV4	19790	26936	1.29%	0.125%
25	11.316	1565	1569	1572	rBV	2363663	1936390	92.70%	8.958%
26	11.380	1576	1580	1583	rVB5	23413	30754	1.47%	0.142%
27	11.851	1656	1660	1673	rBV	1190463	1146245	54.87%	5.303%
28	12.027	1687	1690	1694	rVB2	20891	24535	1.17%	0.114%
29	12.415	1752	1756	1760	rVB3	30479	32616	1.56%	0.151%
30	12.539	1774	1777	1778	rBV	52783	53112	2.54%	0.246%
31	12.557	1778	1780	1786	rVB3	41473	46629	2.23%	0.216%
32	12.633	1790	1793	1801	rBV	702355	697494	33.39%	3.227%
33	12.898	1835	1838	1842	rVB	1019062	829807	39.72%	3.839%
34	13.121	1873	1876	1883	rVB7	17094	33531	1.61%	0.155%

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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	13.368	1914	1918	1924	rVB6	15746	28883	1.38%	0.134%
36	13.486	1936	1938	1945	rVB4	22179	31807	1.52%	0.147%
37	13.809	1988	1993	2000	rBV	363144	513455	24.58%	2.375%
38	13.951	2013	2017	2021	rBV	2013267	1706751	81.71%	7.896%
39	14.133	2045	2048	2052	rBV	69472	64037	3.07%	0.296%
40	14.439	2096	2100	2105	rBV	128359	143612	6.88%	0.664%
41	14.739	2148	2151	2154	rVB	157090	137013	6.56%	0.634%
42	15.068	2203	2207	2211	rBV	166295	174370	8.35%	0.807%
43	15.392	2256	2262	2267	rBV	1183961	1484403	71.06%	6.867%
44	15.439	2267	2270	2275	rVB	151066	190930	9.14%	0.883%
45	15.862	2338	2342	2347	rVB2	124034	179682	8.60%	0.831%
46	15.921	2348	2352	2353	rBV4	34805	45343	2.17%	0.210%
47	16.356	2421	2426	2431	rVB4	72678	119444	5.72%	0.553%

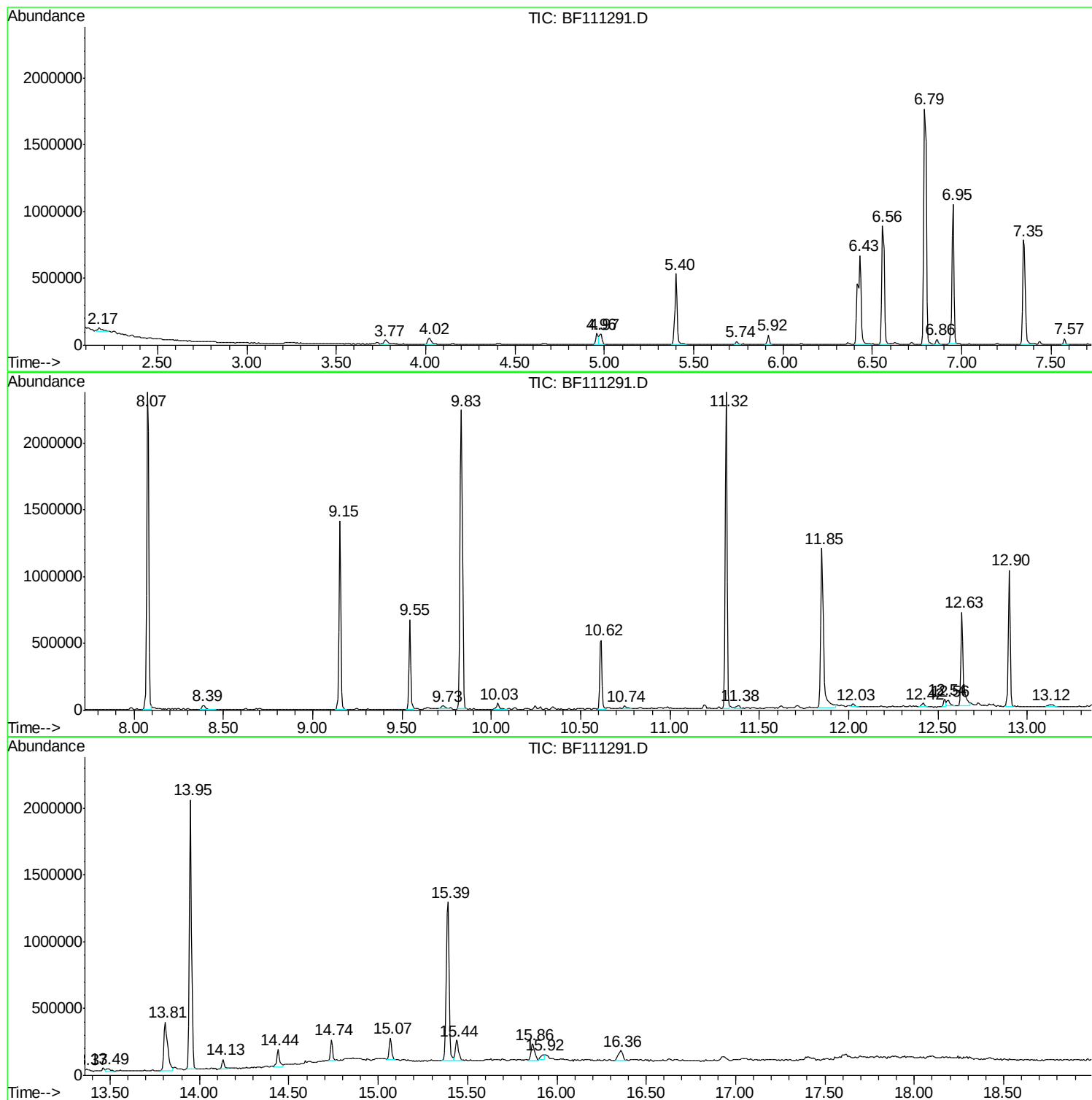
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF120818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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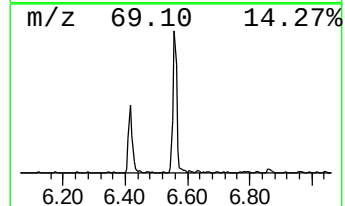
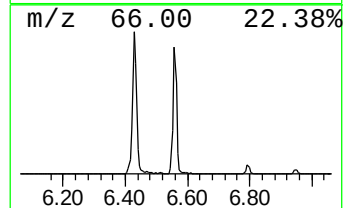
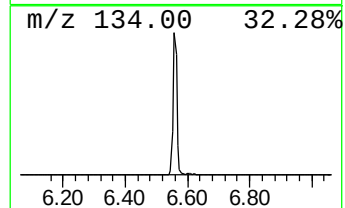
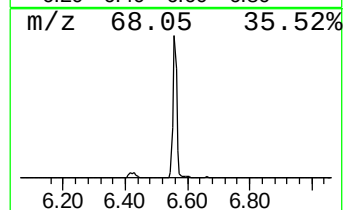
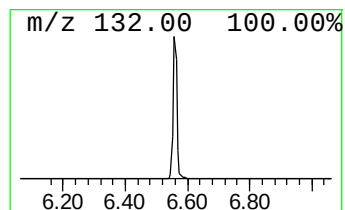
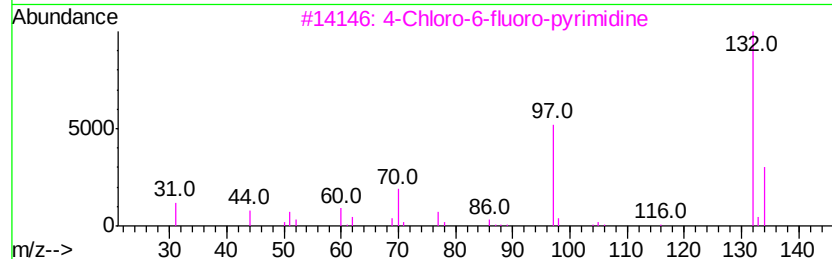
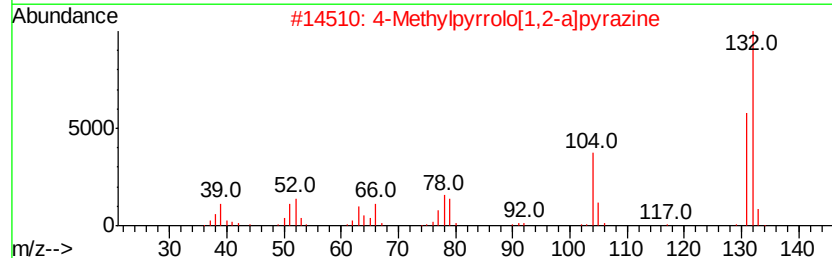
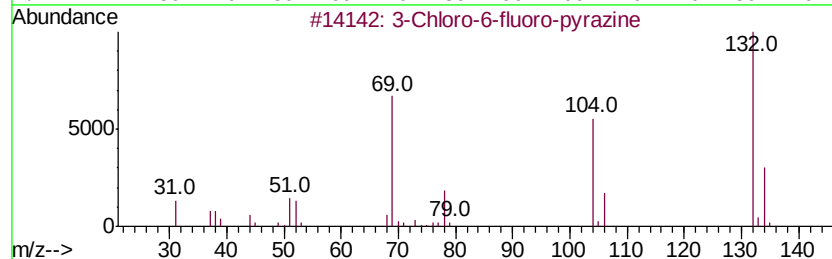
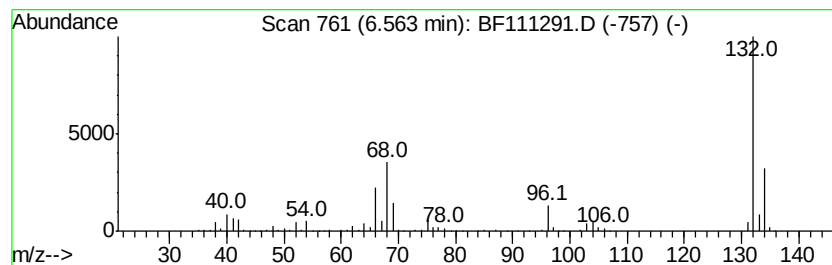
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF120818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown6.56 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	9.85 ng	760207	1,4-Dichlorobenzene-d4	6.79

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2			4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
3			4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
4			1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5			Amphetaminil	250	C17H18N2	017590-01-1	9



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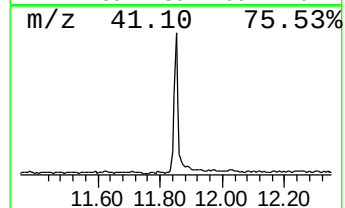
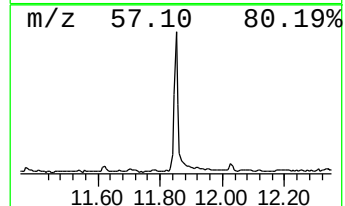
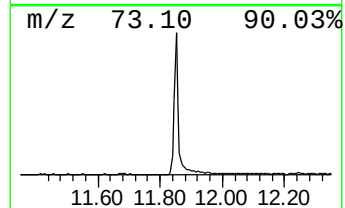
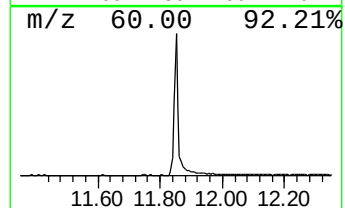
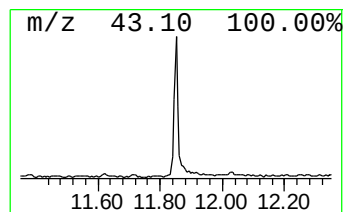
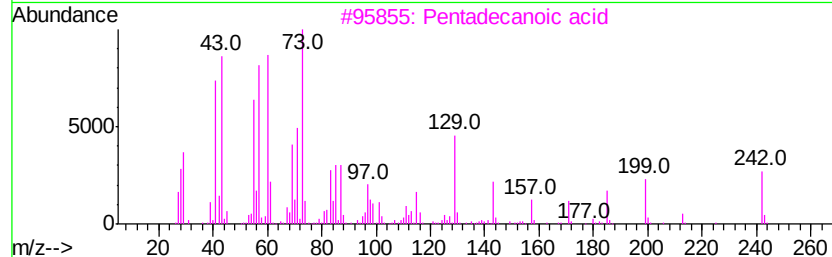
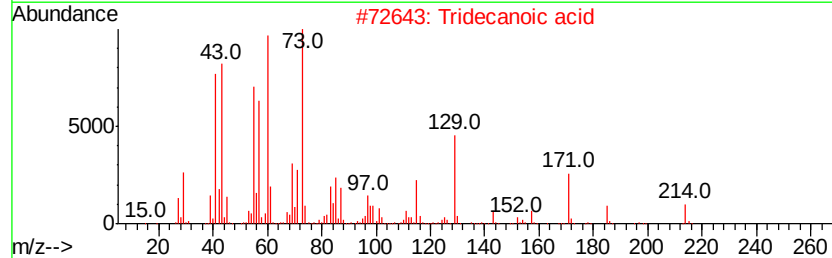
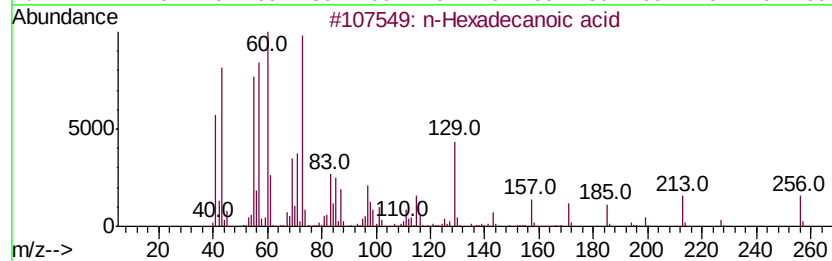
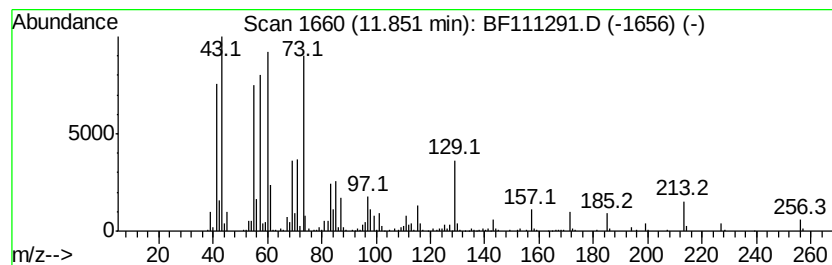
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.85	11.84 ng	1146250	Phenanthrene-d10		11.32
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Dodecanoic acid	200	C12H24O2	000143-07-7	64
5	Undecanoic acid	186	C11H22O2	000112-37-8	64



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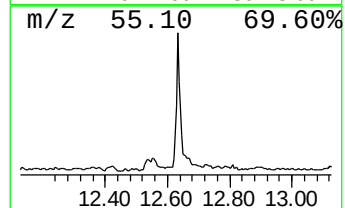
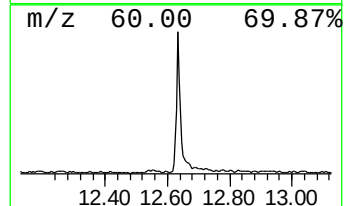
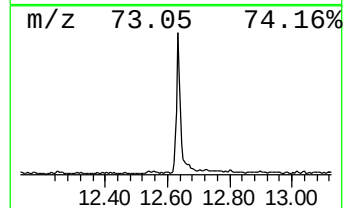
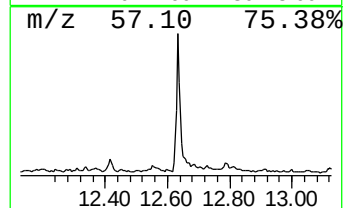
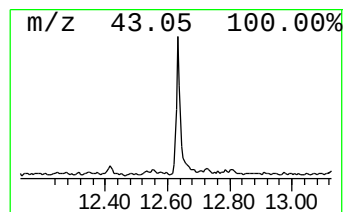
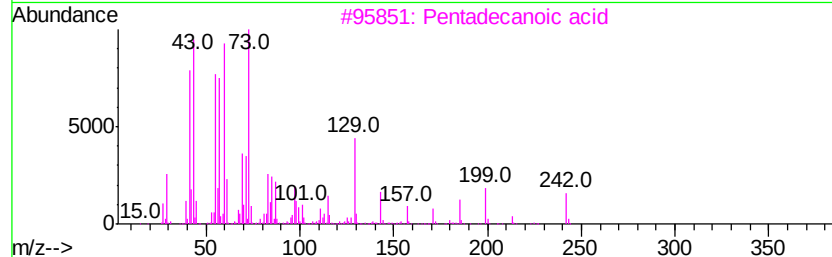
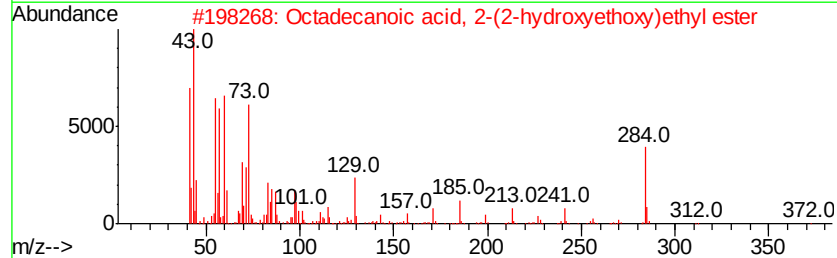
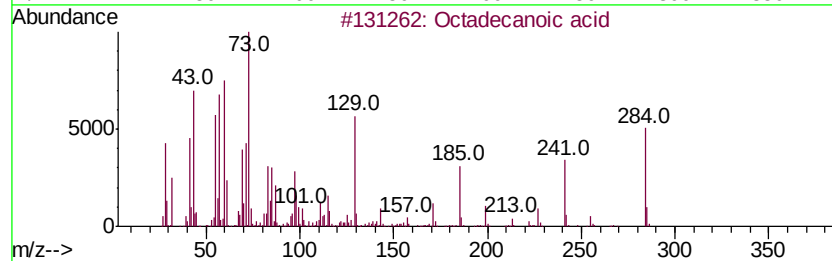
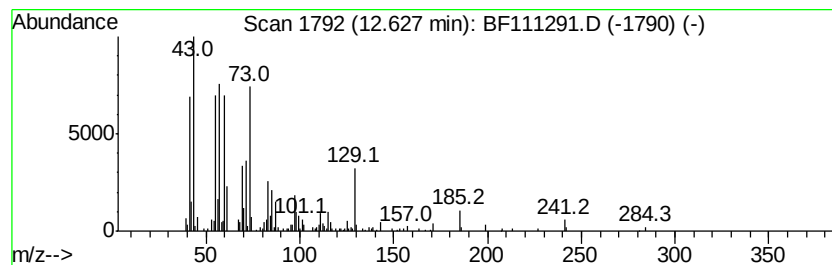
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF120818.M
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.63	7.20 ng	697494	Phenanthrene-d10	11.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		Octadecanoic acid, 2-(2-hydroxyve...	372	C22H44O4	000106-11-6	87
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	80
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5		Tridecanoic acid	214	C13H26O2	000638-53-9	64



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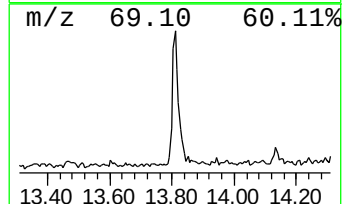
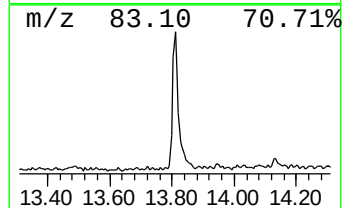
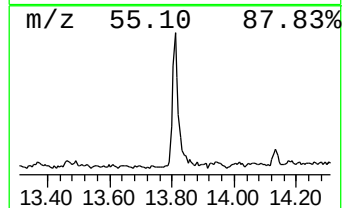
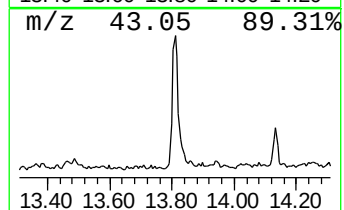
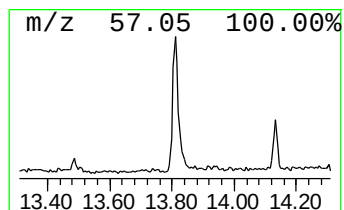
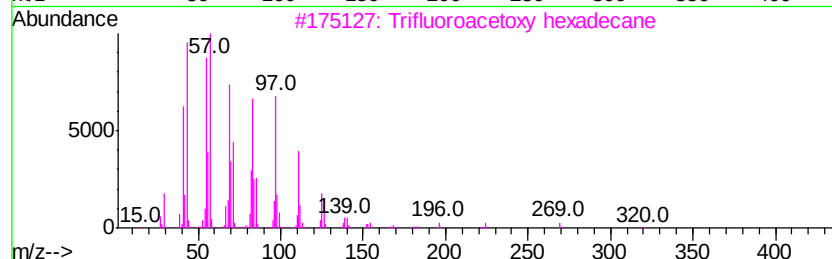
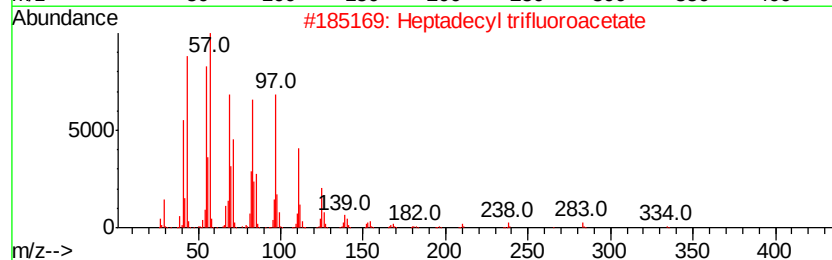
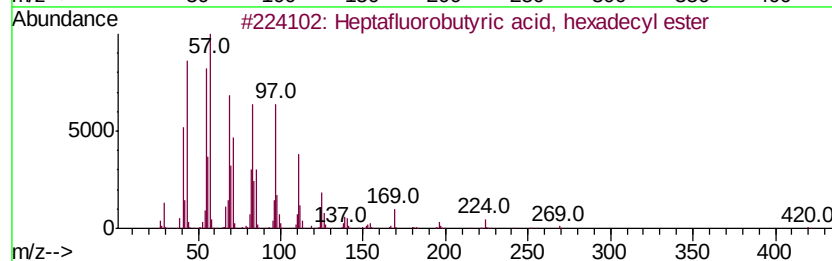
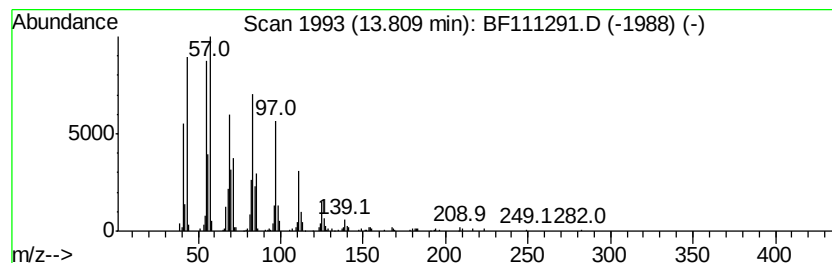
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Heptafluorobutyric acid, he... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.81	6.02 ng	513455	Chrysene-d12	13.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	94
2		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	94
3		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
4		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
5		1-Docosene	308	C22H44	001599-67-3	94



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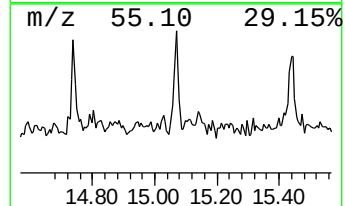
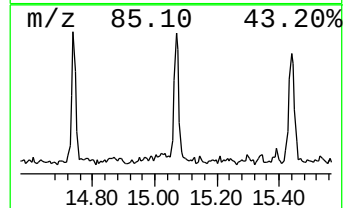
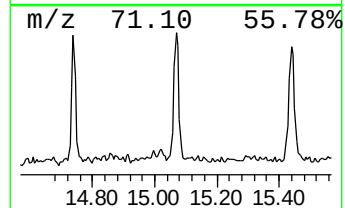
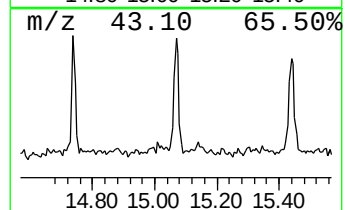
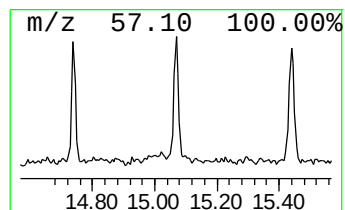
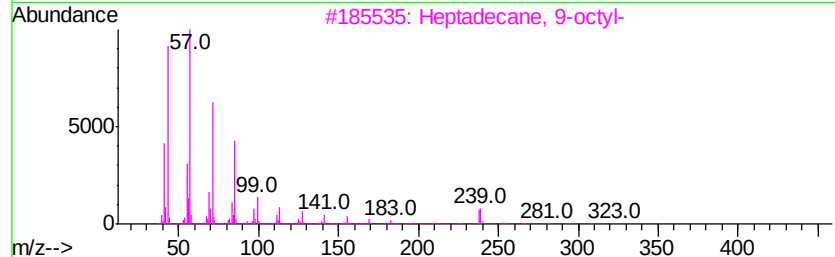
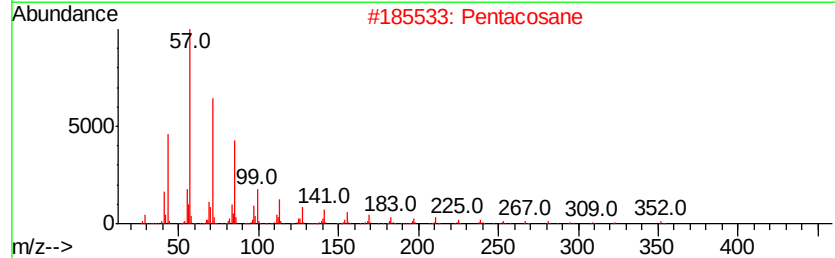
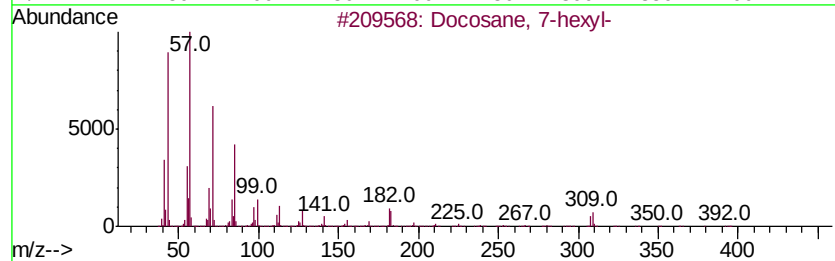
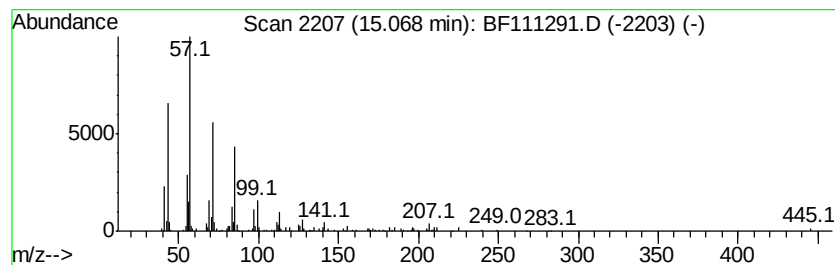
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Docosane, 7-hexyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.07	2.35 ng	174370	Perylene-d12	15.39

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Docosane, 7-hexyl-	394	C28H58	055373-86-9	87
2		Pentacosane	352	C25H52	000629-99-2	87
3		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
4		Eicosane, 7-hexyl-	366	C26H54	055333-99-8	87
5		Hexacosane	366	C26H54	000630-01-3	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121118\
Data File : BF111291.D
Acq On : 11 Dec 2018 22:18
Operator : JU/SJ
Sample : J6157-09
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSITE-5-TOTAL

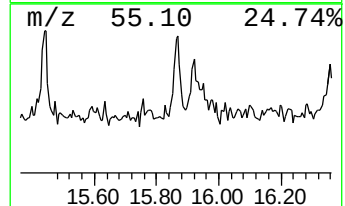
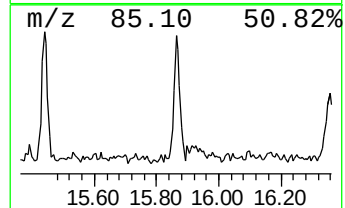
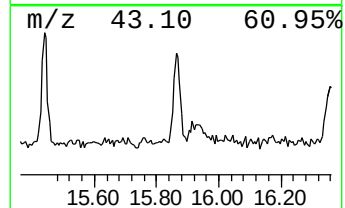
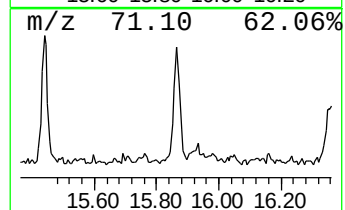
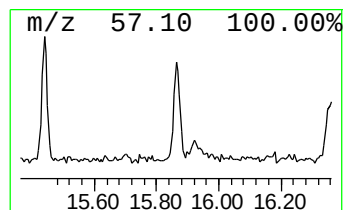
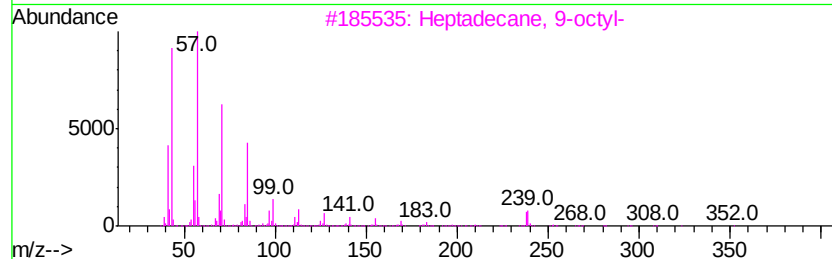
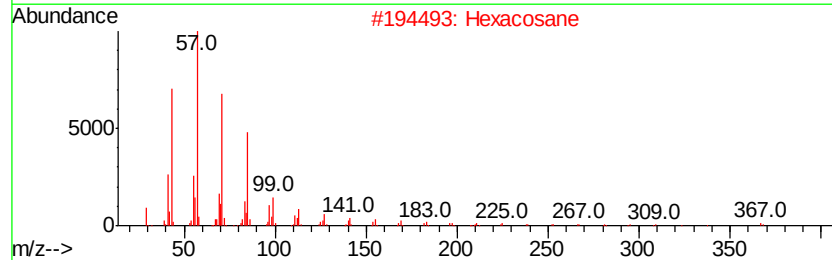
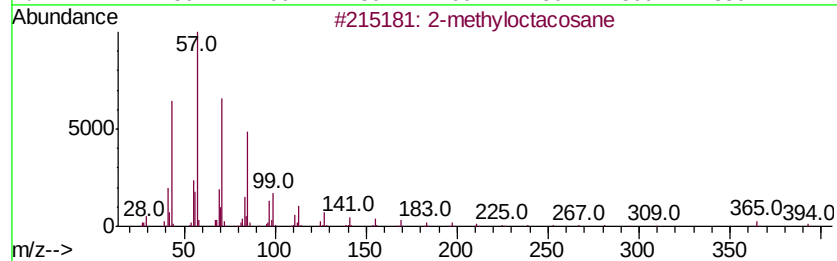
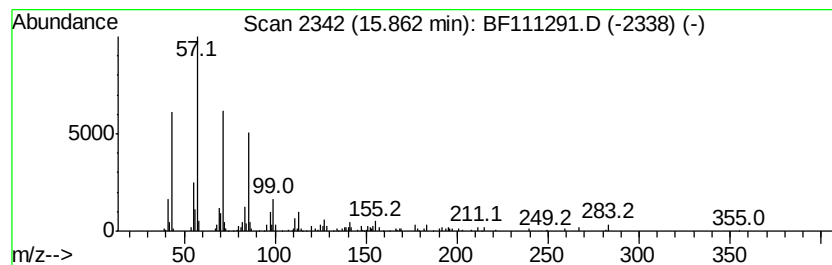
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 2-methyloctacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.86	2.42 ng	179682	Perylene-d12	15.39

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-methyloctacosane	408	C29H60	1000376-72-8	87
2		Hexacosane	366	C26H54	000630-01-3	86
3		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	86
4		Hentriacontane	437	C31H64	000630-04-6	68
5		Hexatriacontane	507	C36H74	000630-06-8	68



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF121118\
Data File : BF111291.D
Acq On : 11 Dec 2018 22:18
Operator : JU/SJ
Sample : J6157-09
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSITE-5-TOTAL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120818.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
unknown6.56	6.56	9.8	ng	760207	1	6.79	1544150	20.0
n-Hexadecanoic acid	11.85	11.8	ng	1146250	4	11.32	1936390	20.0
Octadecanoic acid	12.63	7.2	ng	697494	4	11.32	1936390	20.0
Heptafluorobutyri...	13.81	6.0	ng	513455	5	13.95	1706750	20.0
Docosane, 7-hexyl-	15.07	2.4	ng	174370	6	15.39	1484400	20.0
2-methyloctacosane	15.86	2.4	ng	179682	6	15.39	1484400	20.0