

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081518\
 Data File : BF108161.D
 Acq On : 15 Aug 2018 13:10
 Operator : JU/SJ
 Sample : J4447-26
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SP-1-9

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-BF080818.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	5.260	492	497	504	rBV	671363	782929	17.17%	2.002%
2	5.648	558	563	566	rBV	3881080	3647333	79.99%	9.327%
3	6.637	726	731	735	rBV	3584948	3941834	86.45%	10.080%
4	6.790	752	757	760	rBV	4218500	3871565	84.91%	9.900%
5	7.019	792	796	799	rBV	1324838	1090711	23.92%	2.789%
6	7.172	818	822	826	rBV	3292458	2978907	65.33%	7.617%
7	7.578	886	891	894	rBV	2661141	2534126	55.58%	6.480%
8	8.301	1010	1014	1017	rBV	1695996	1380337	30.27%	3.530%
9	9.372	1191	1196	1200	rBV	4767189	4559529	100.00%	11.659%
10	9.760	1259	1262	1266	rBV	471403	425618	9.33%	1.088%
11	10.066	1309	1314	1318	rBV	1558085	1544786	33.88%	3.950%
12	10.378	1362	1367	1371	rBV	32111	51394	1.13%	0.131%
13	10.854	1444	1448	1452	rBV	2698092	2666839	58.49%	6.819%
14	10.960	1461	1466	1470	rBV2	83025	129683	2.84%	0.332%
15	11.395	1538	1540	1543	rBV	64691	58257	1.28%	0.149%
16	11.560	1564	1568	1571	rBV	1717124	1442401	31.63%	3.688%
17	11.824	1610	1613	1616	rBV	58898	50478	1.11%	0.129%
18	12.060	1650	1653	1656	rBV	149673	149483	3.28%	0.382%
19	12.777	1773	1775	1779	rVB	67792	62236	1.36%	0.159%
20	13.013	1810	1815	1821	rBV2	72211	105430	2.31%	0.270%
21	13.148	1834	1838	1841	rBV	4156461	3709504	81.36%	9.486%
22	14.030	1984	1988	1995	rBV	353859	378688	8.31%	0.968%
23	14.213	2016	2019	2023	rBV	1312995	1208502	26.50%	3.090%
24	14.348	2039	2042	2046	rBV	73555	68200	1.50%	0.174%
25	14.671	2092	2097	2103	rVB2	135837	240177	5.27%	0.614%
26	14.983	2148	2150	2154	rVB	93104	97513	2.14%	0.249%
27	15.071	2161	2165	2169	rBV	165344	185225	4.06%	0.474%
28	15.354	2210	2213	2216	rVB	142712	156199	3.43%	0.399%
29	15.783	2280	2286	2290	rBV	981286	1381812	30.31%	3.533%
30	16.248	2362	2365	2372	rVB	144714	206940	4.54%	0.529%

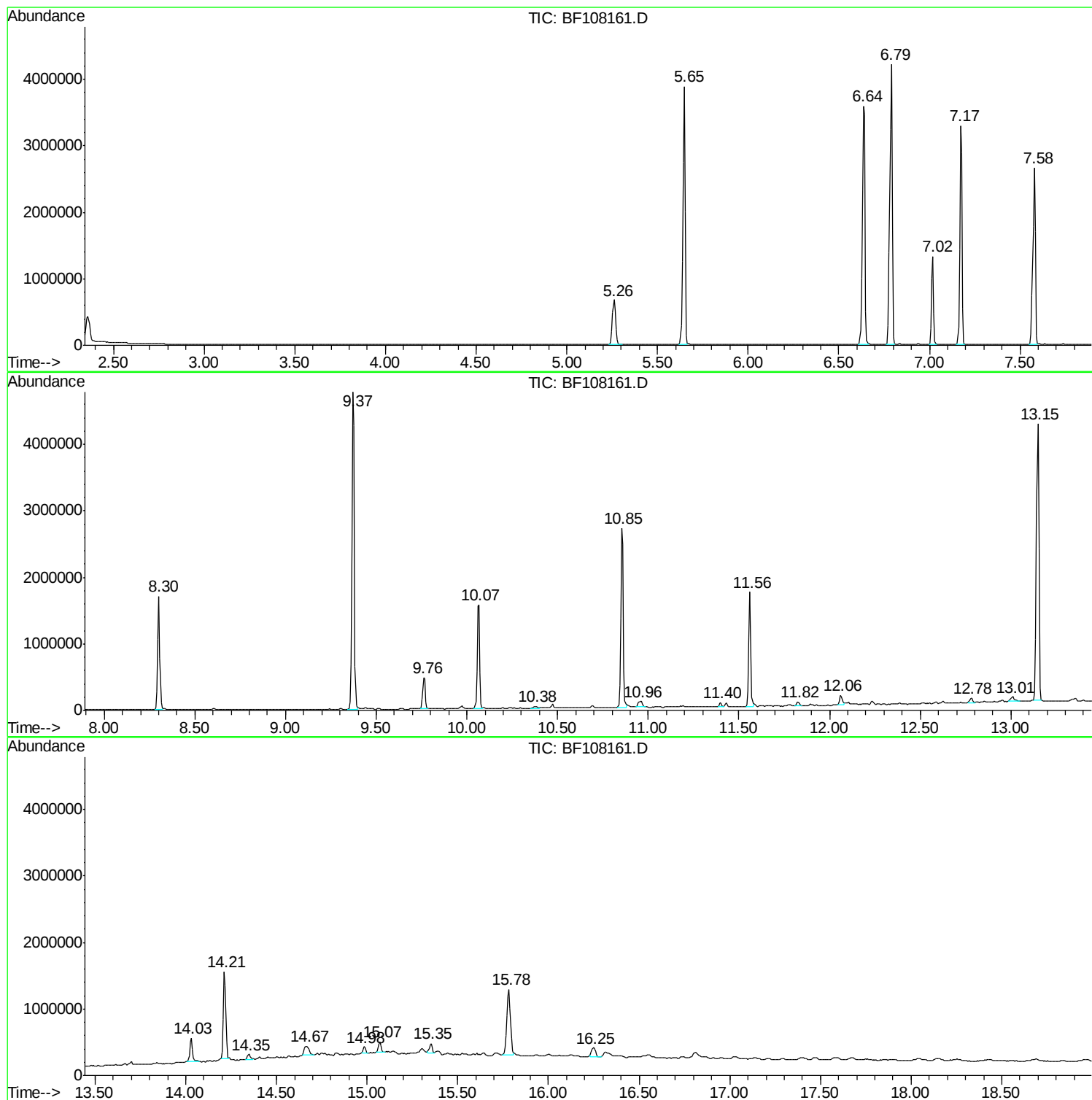
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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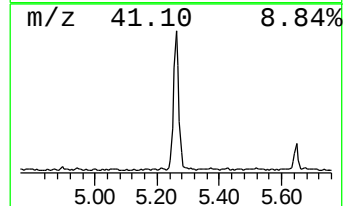
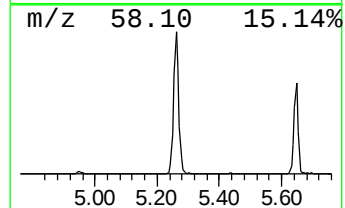
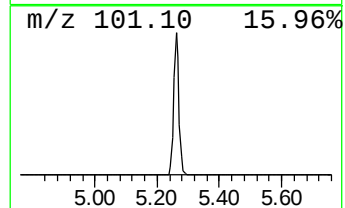
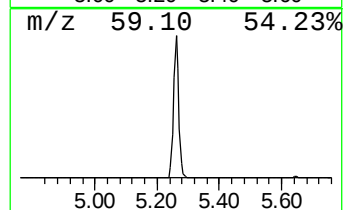
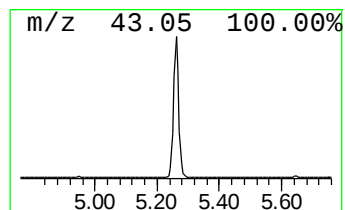
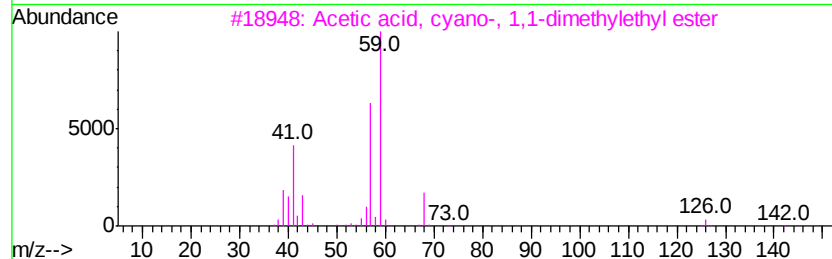
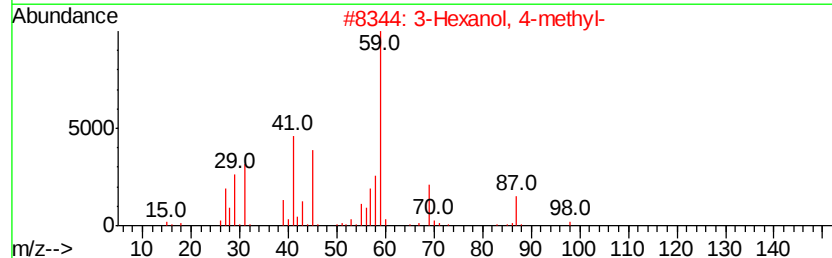
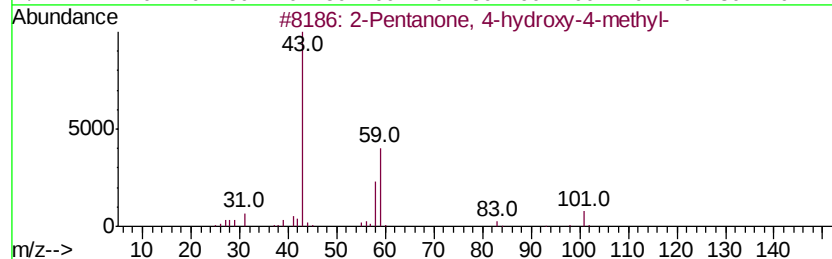
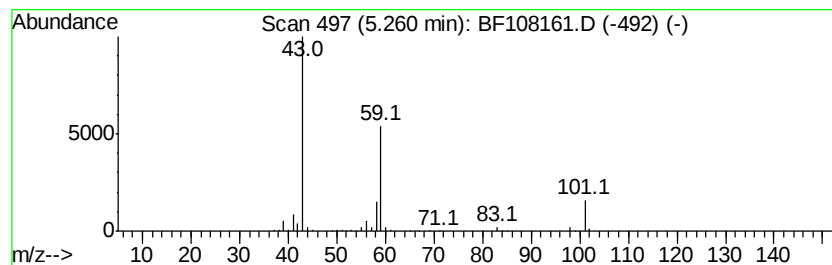
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.26	14.36 ng	782929	1,4-Dichlorobenzene-d4	7.02

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	32
4			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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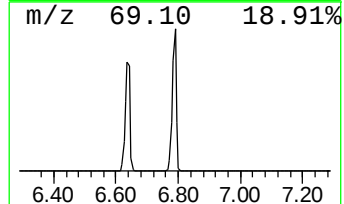
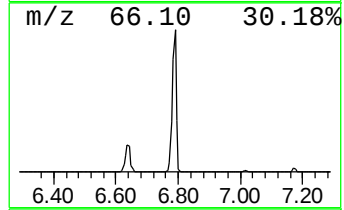
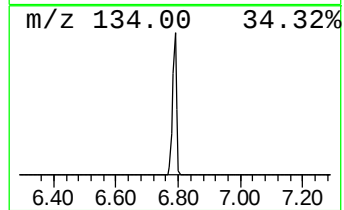
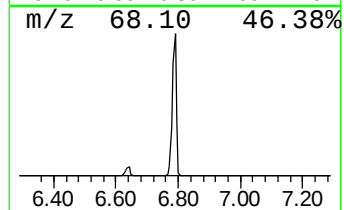
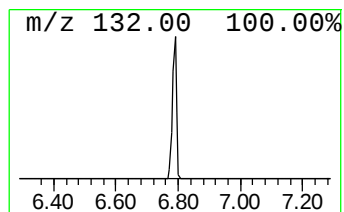
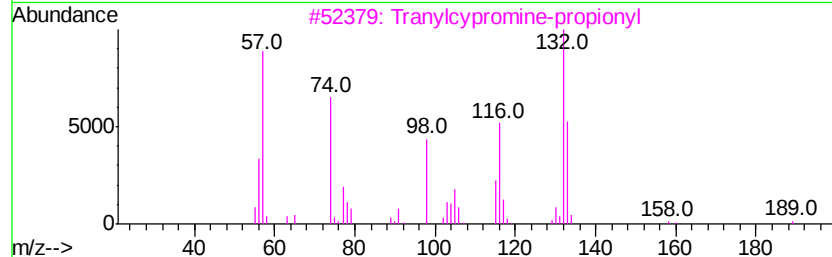
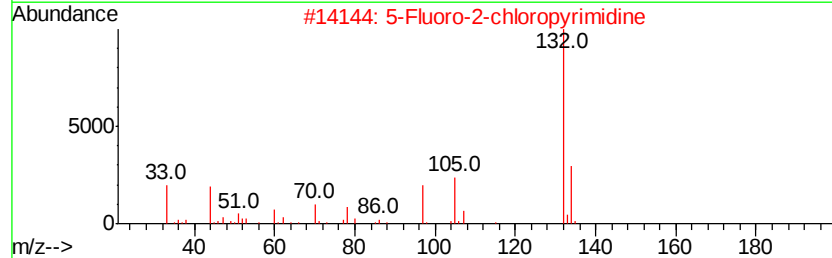
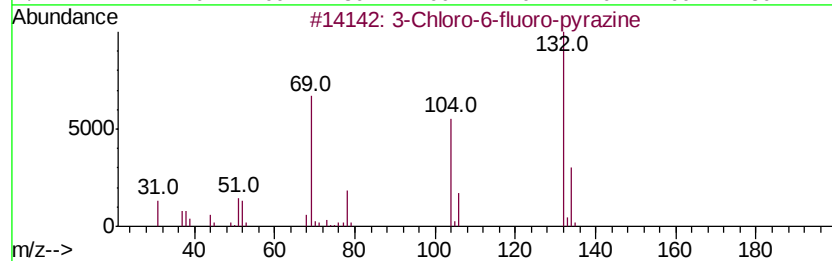
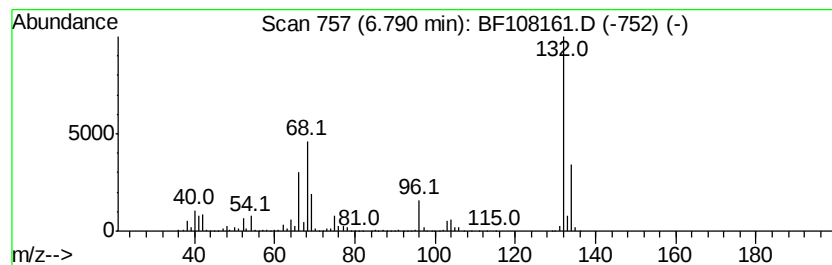
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Peak Number 2 unknown6.79 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.79	70.99 ng	3871570	1,4-Dichlorobenzene-d4	7.02

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
5		1,2,4-Trifluorobenzene	132	C6H3F3	000367-23-7	9



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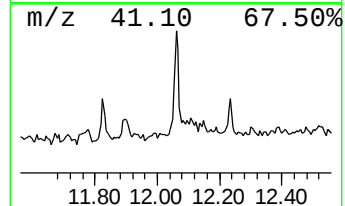
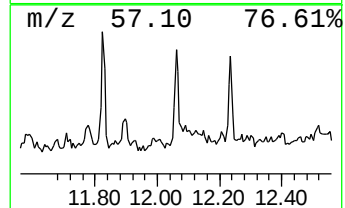
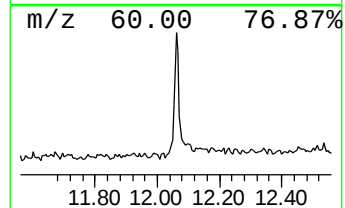
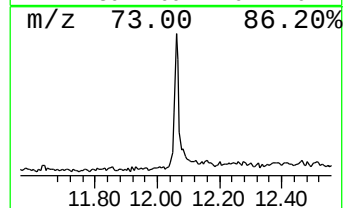
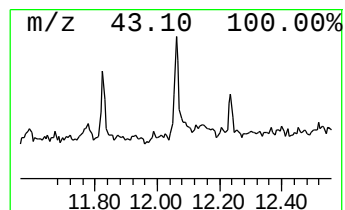
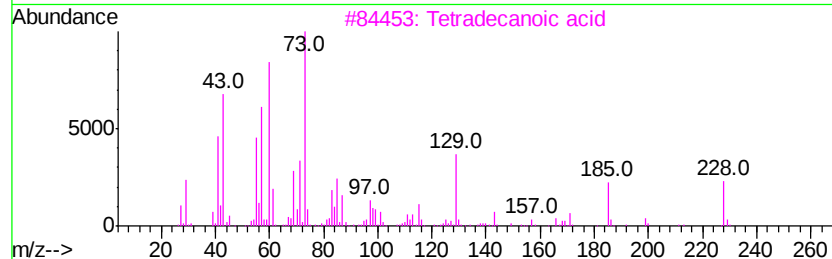
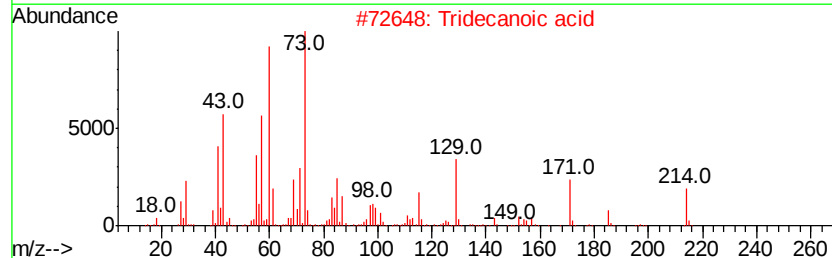
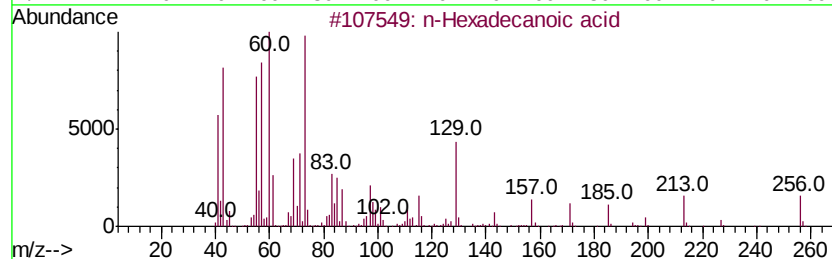
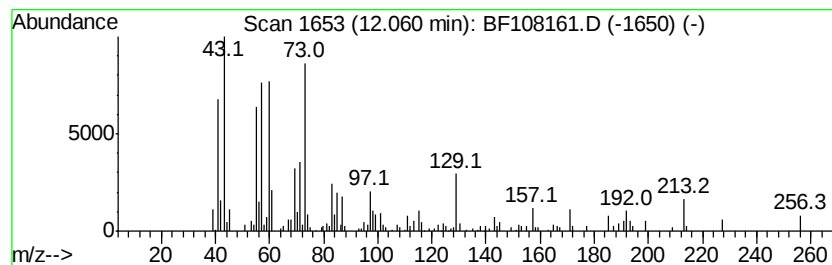
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.06	2.07 ng	149483	Phenanthrene-d10	11.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	76
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	72
5	Dodecanoic acid	200	C12H24O2	000143-07-7	64



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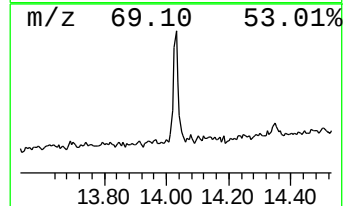
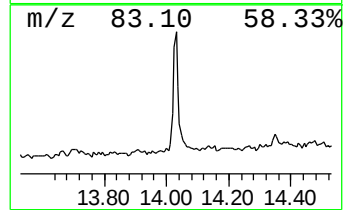
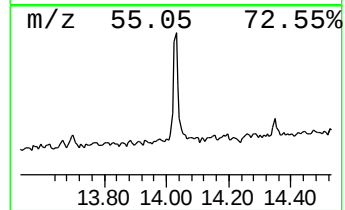
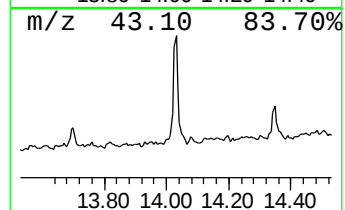
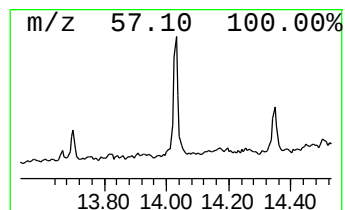
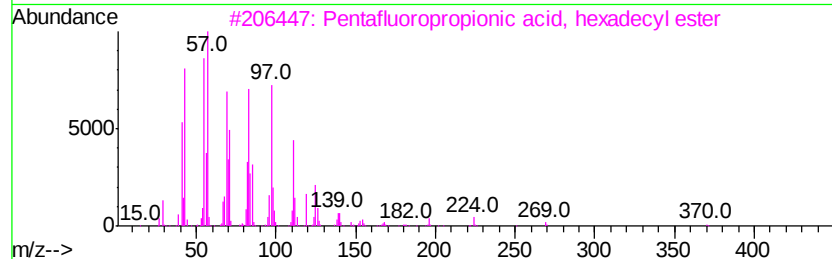
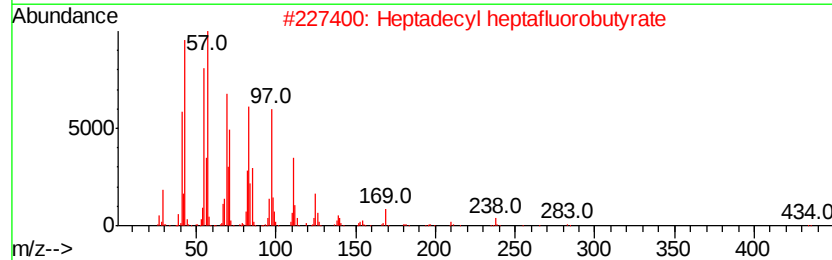
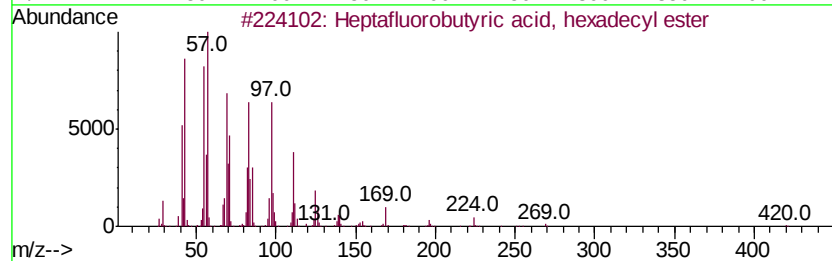
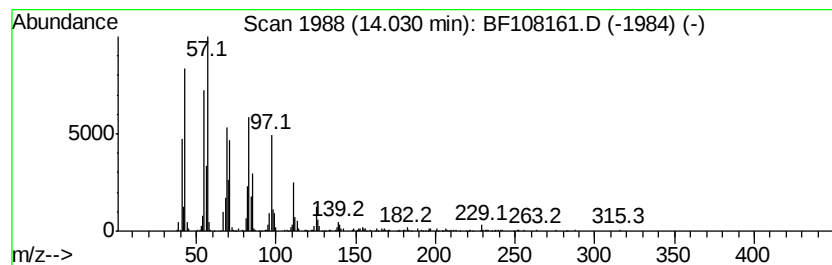
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Peak Number 5 Heptafluorobutyric acid, he... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.03	6.27 ng	378688	Chrysene-d12	14.21

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	94
2		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
3		Pentafluoropropionic acid, hexadec...	388	C19H33F5O2	006222-07-7	91
4		Heptafluorobutyric acid, n-octadec...	466	C22H37F7O2	000400-57-7	91
5		Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91



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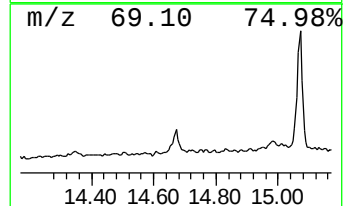
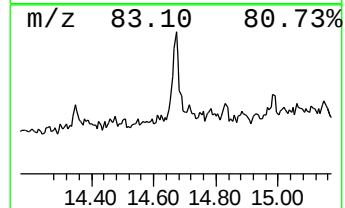
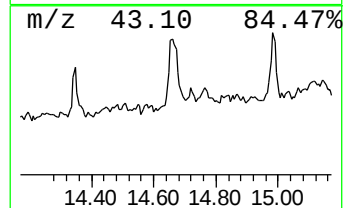
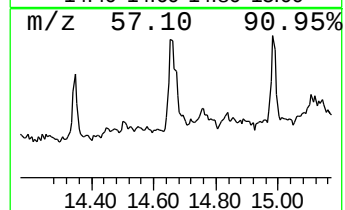
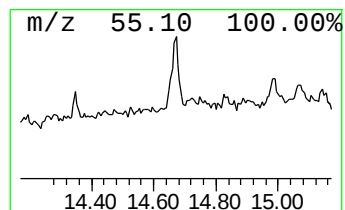
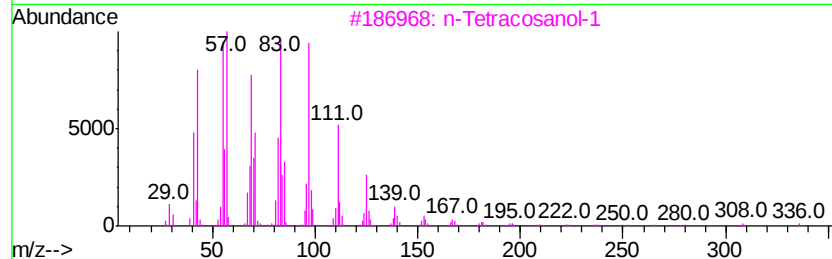
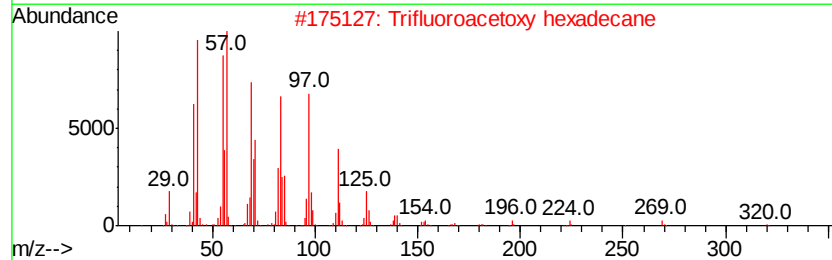
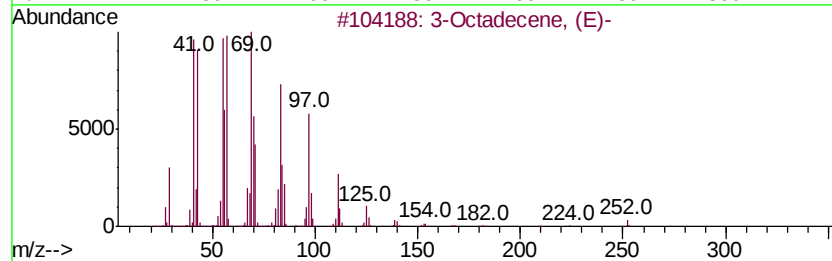
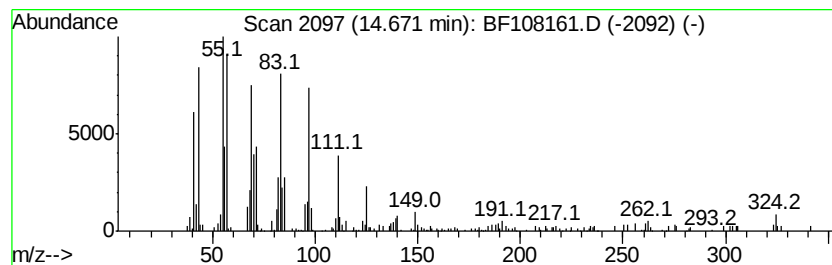
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Peak Number 6 3-Octadecene, (E)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.67	3.97 ng	240177	Chrysene-d12	14.21

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Octadecene, (E)-	252	C18H36	007206-19-1	91
2		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
3		n-Tetracosanol-1	354	C24H50O	000506-51-4	87
4		3-Eicosene, (E)-	280	C20H40	074685-33-9	83
5		1-Heneicosyl formate	340	C22H44O2	077899-03-7	83



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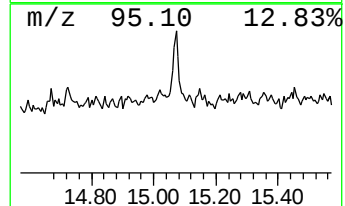
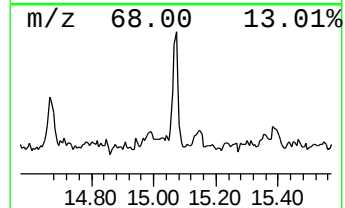
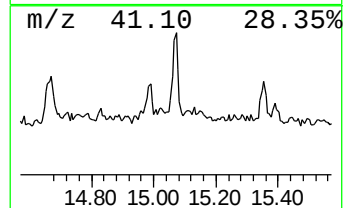
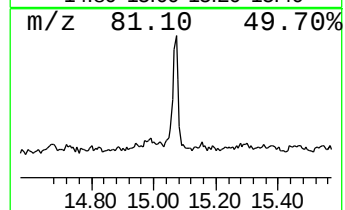
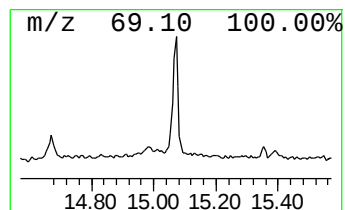
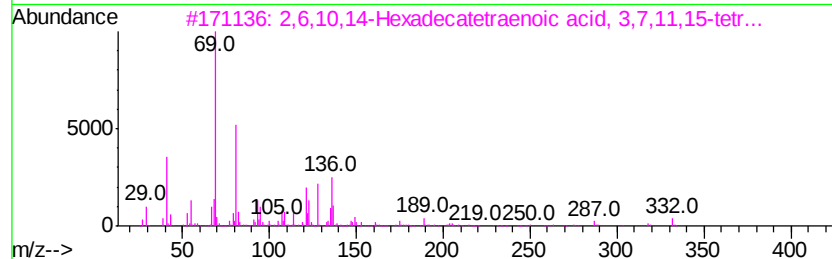
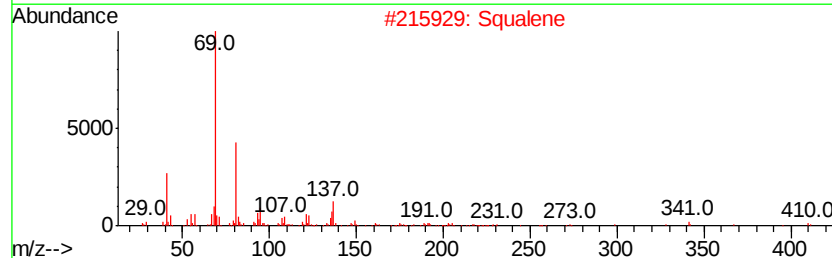
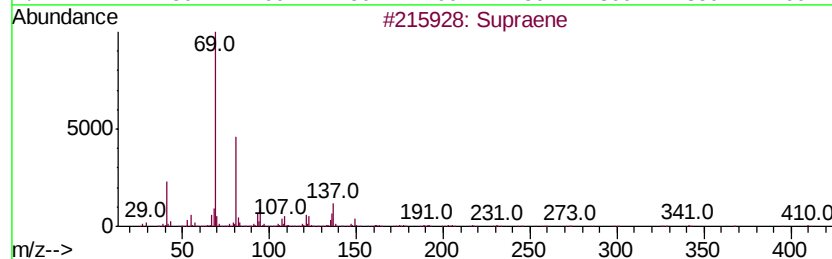
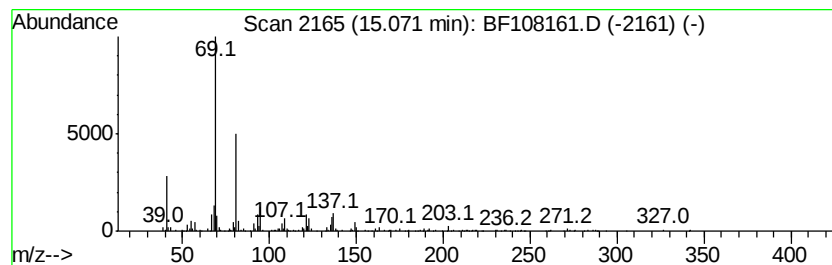
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Supraene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.07	2.68 ng	185225	Perylene-d12	15.78

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Supraene	410	C30H50	007683-64-9	91
2		Squalene	410	C30H50	000111-02-4	90
3		2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	72
4		1,5,9-Decatriene, 2,3,5,8-tetram...	192	C14H24	230646-72-7	64
5		1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	50



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081518\
Data File : BF108161.D
Acq On : 15 Aug 2018 13:10
Operator : JU/SJ
Sample : J4447-26
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-1-9

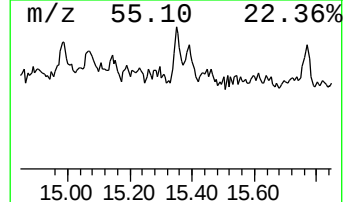
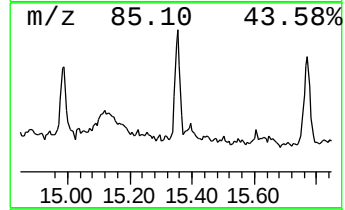
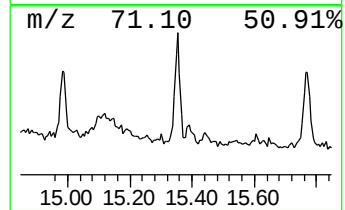
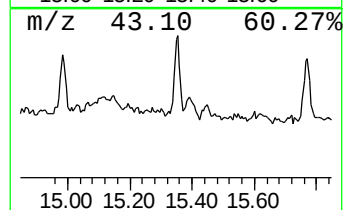
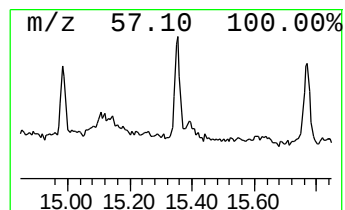
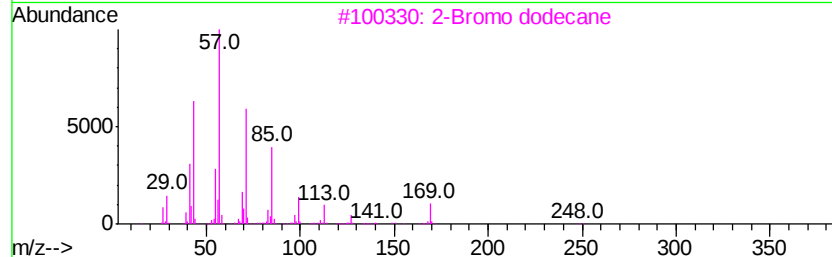
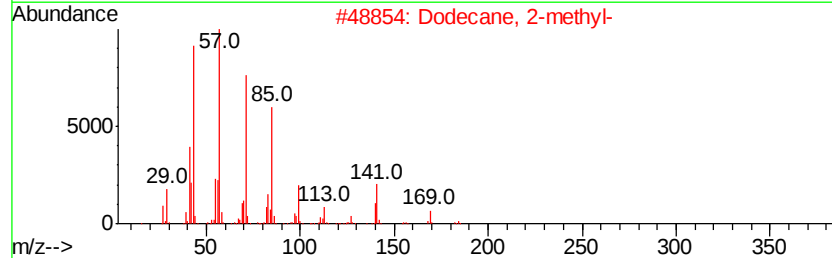
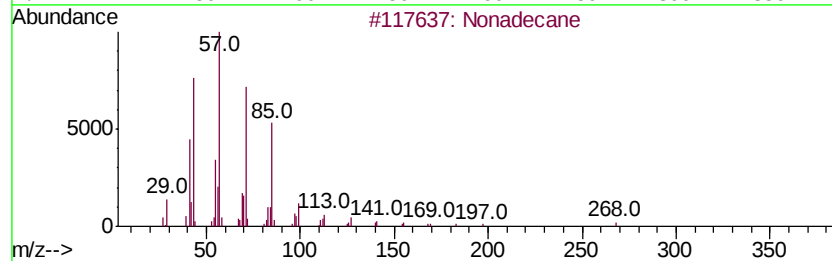
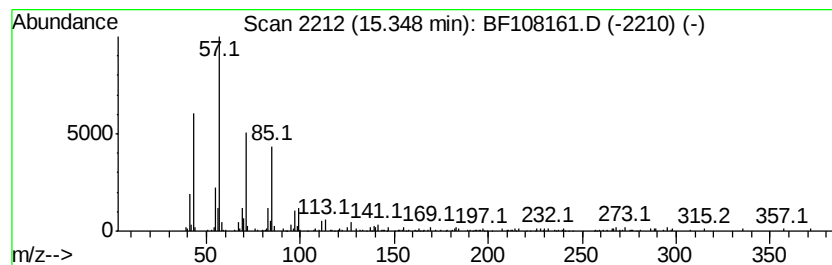
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Nonadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.35	2.26 ng	156199	Perylene-d12	15.78

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane		268	C19H40	000629-92-5	81
2	Dodecane, 2-methyl-		184	C13H28	001560-97-0	80
3	2-Bromo dodecane		248	C12H25Br	013187-99-0	80
4	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	80
5	Tridecane, 1-iodo-		310	C13H27I	035599-77-0	80



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081518\
Data File : BF108161.D
Acq On : 15 Aug 2018 13:10
Operator : JU/SJ
Sample : J4447-26
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-1-9

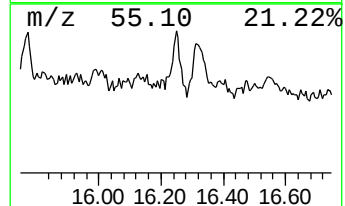
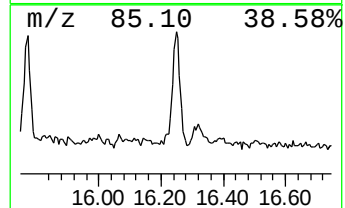
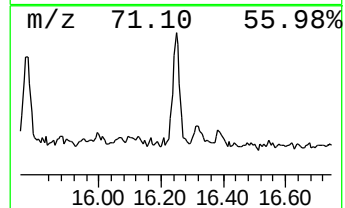
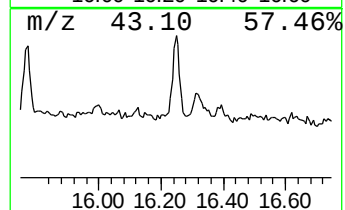
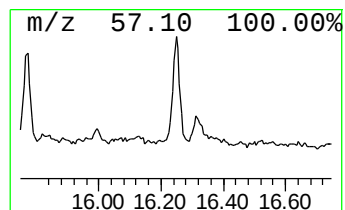
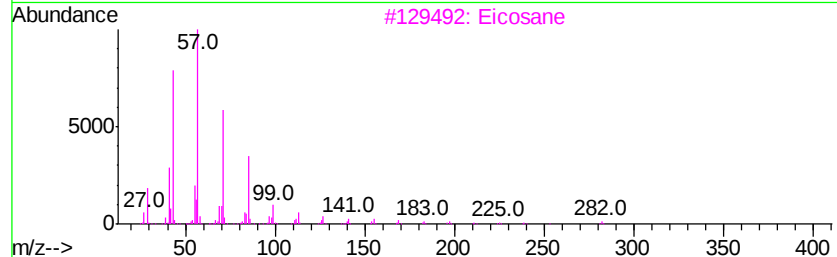
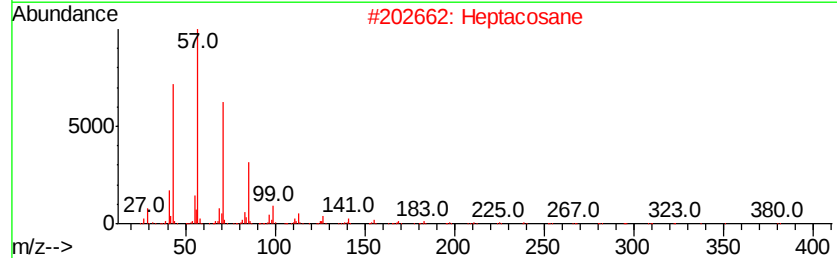
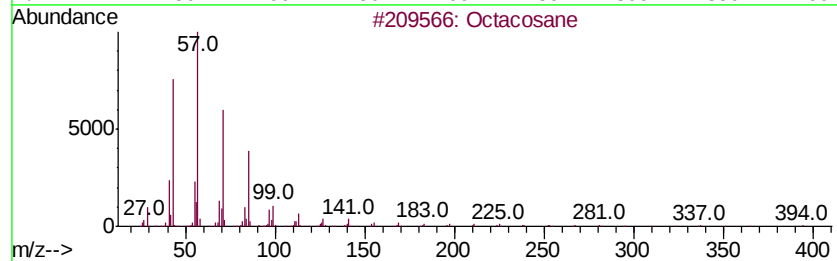
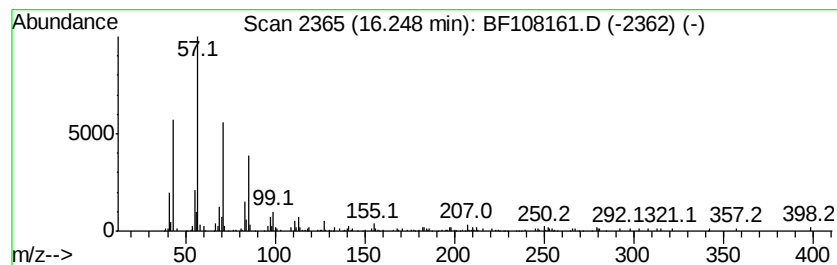
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Octacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.25	3.00 ng	206940	Perylene-d12	15.78

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	87
2		Heptacosane	380	C27H56	000593-49-7	83
3		Eicosane	282	C20H42	000112-95-8	80
4		Tridecane, 2-methyl-	198	C14H30	001560-96-9	80
5		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	74



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF081518\
Data File : BF108161.D
Acq On : 15 Aug 2018 13:10
Operator : JU/SJ
Sample : J4447-26
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-1-9

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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...	5.26	14.4	ng	782929	1	7.02	1090710	20.0
unknown6.79	6.79	71.0	ng	3871570	1	7.02	1090710	20.0
n-Hexadecanoic acid	12.06	2.1	ng	149483	4	11.56	1442400	20.0
Heptafluorobutyri...	14.03	6.3	ng	378688	5	14.21	1208500	20.0
3-Octadecene, (E)-	14.67	4.0	ng	240177	5	14.21	1208500	20.0
Supraene	15.07	2.7	ng	185225	6	15.78	1381810	20.0
Nonadecane	15.35	2.3	ng	156199	6	15.78	1381810	20.0
Octacosane	16.25	3.0	ng	206940	6	15.78	1381810	20.0