

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF121518\
 Data File : BF111467.D
 Acq On : 15 Dec 2018 14:35
 Operator : JU/SJ
 Sample : J6322-19
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SUP-5A-C-1-120718

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-BF121418.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	5.010	491	497	509	rVB	167691	243140	4.77%	0.632%
2	5.428	563	568	571	rBV	4406572	4401136	86.43%	11.446%
3	6.439	735	740	757	rBV	4312649	5092202	100.00%	13.243%
4	6.569	757	762	765	rBV	5045772	4656085	91.44%	12.109%
5	6.792	796	800	807	rBV	1180407	951693	18.69%	2.475%
6	6.951	823	827	830	rBV	4182098	3641507	71.51%	9.470%
7	7.357	890	896	899	rBV	3167785	3010405	59.12%	7.829%
8	8.075	1014	1018	1035	rBV	1455147	1260960	24.76%	3.279%
9	9.157	1196	1202	1205	rBV	5044028	4988778	97.97%	12.974%
10	9.545	1264	1268	1277	rBV	313642	308686	6.06%	0.803%
11	9.827	1312	1316	1327	rVB	1462063	1303298	25.59%	3.389%
12	10.616	1446	1450	1458	rBV	2218509	2032251	39.91%	5.285%
13	11.310	1564	1568	1575	rBV	1219861	1084602	21.30%	2.821%
14	11.845	1650	1659	1669	rBV	175246	257939	5.07%	0.671%
15	12.627	1787	1792	1803	rBV	102337	160418	3.15%	0.417%
16	12.898	1834	1838	1841	rBV	3471720	3145460	61.77%	8.180%
17	13.804	1987	1992	2005	rBV3	102040	182221	3.58%	0.474%
18	13.945	2012	2016	2027	rBV	837743	866330	17.01%	2.253%
19	14.798	2158	2161	2167	rVB	74953	80484	1.58%	0.209%
20	15.386	2256	2261	2266	rBV	635208	783869	15.39%	2.039%

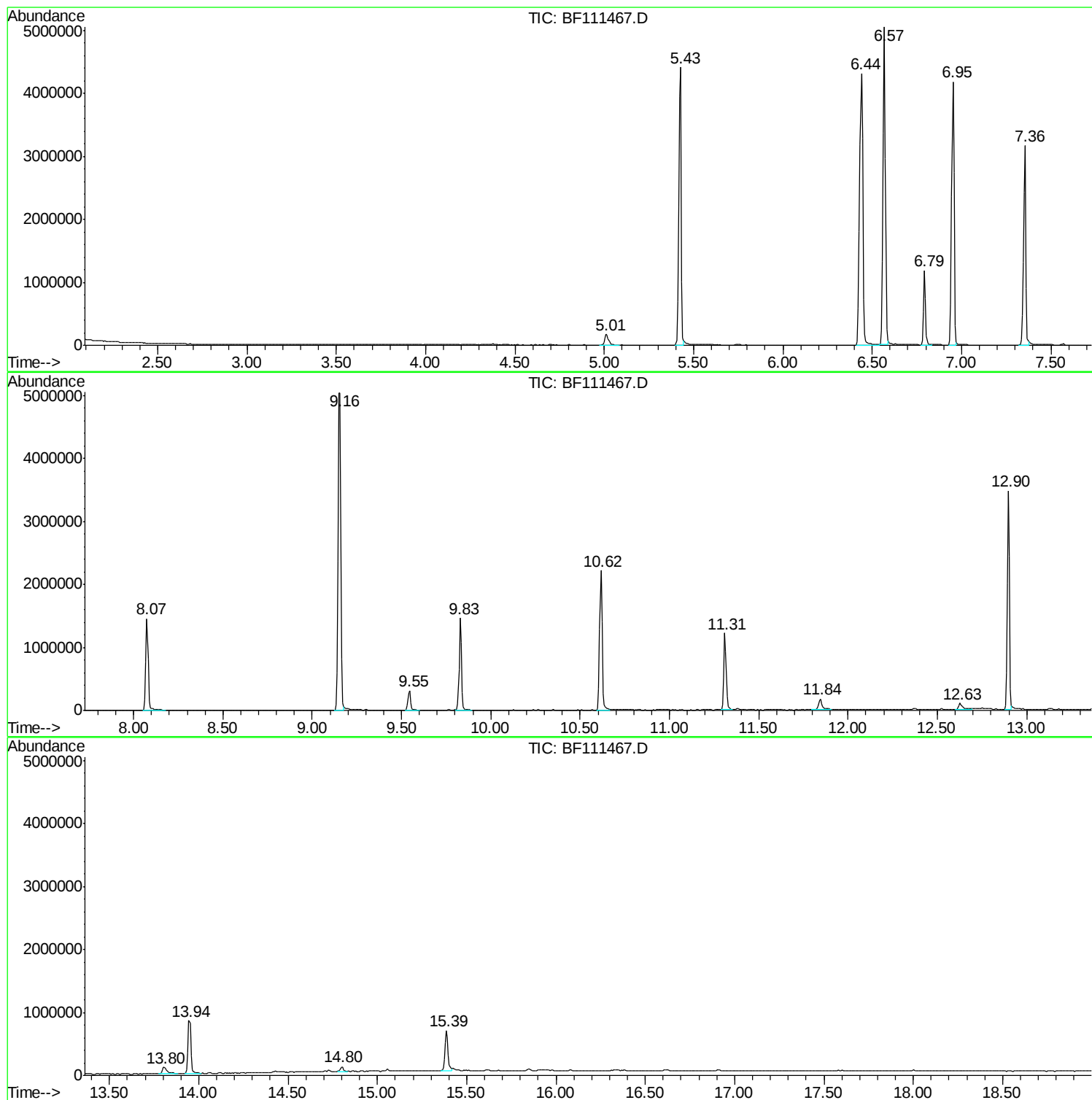
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF121418.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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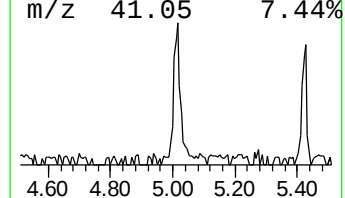
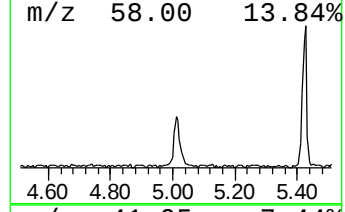
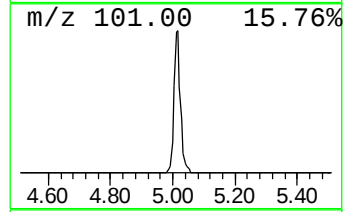
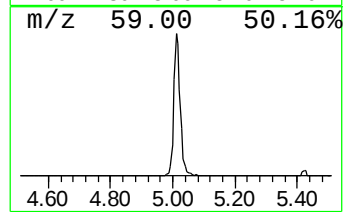
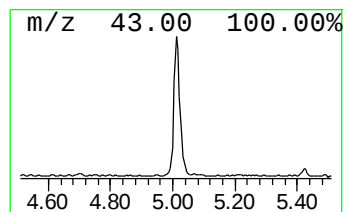
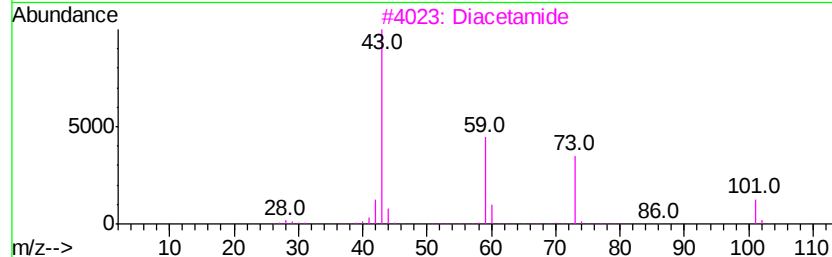
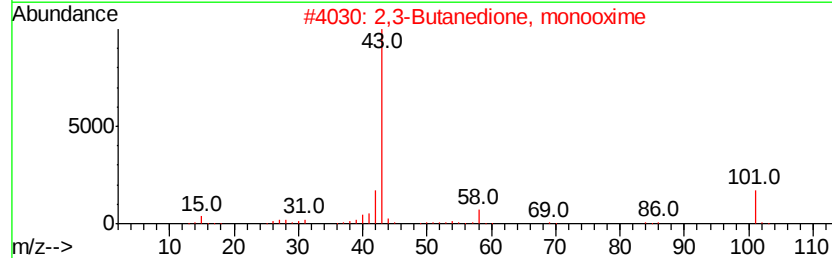
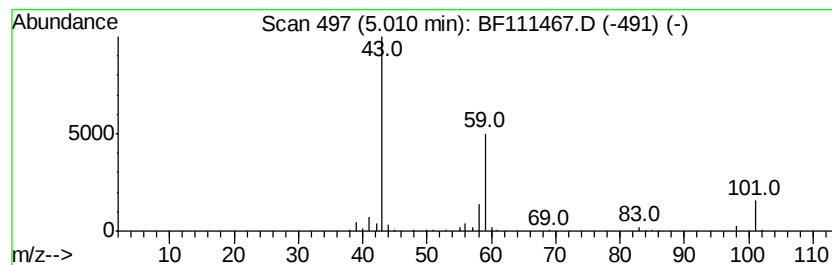
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.01	5.11 ng	243140	1,4-Dichlorobenzene-d4	6.79

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
3			Diacetamide	101	C4H7NO2	000625-77-4	9
4			3,3-Dimethylbutylamine	101	C6H15N	015673-00-4	9
5			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	9



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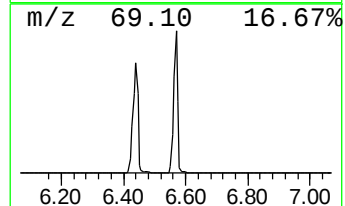
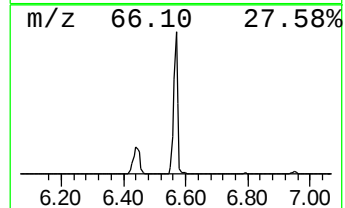
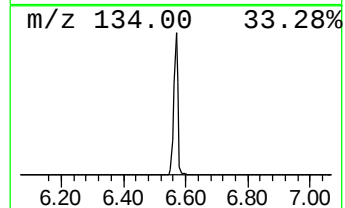
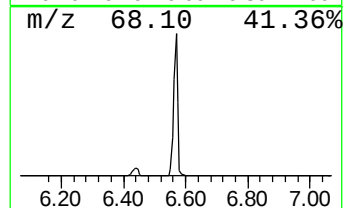
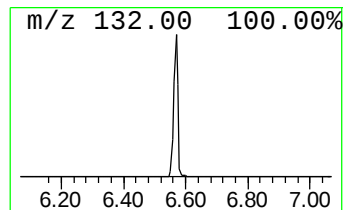
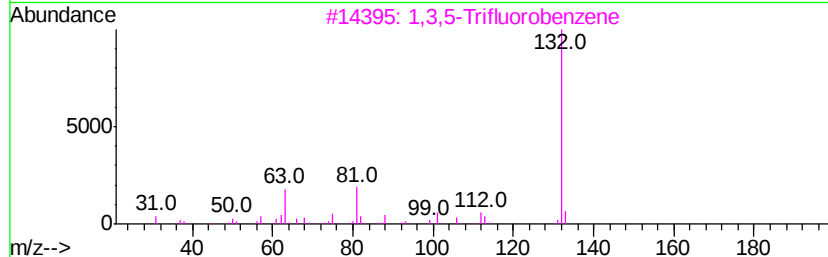
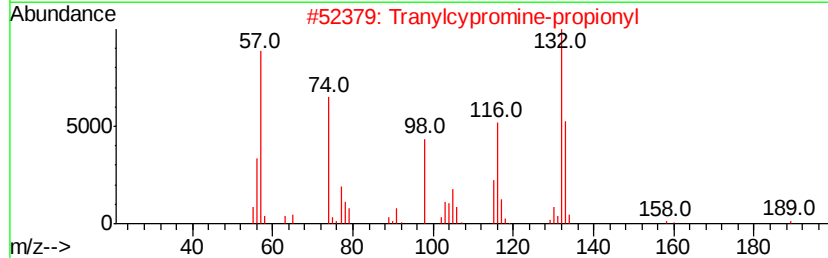
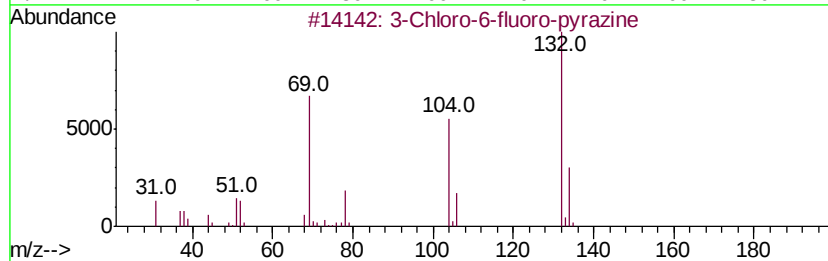
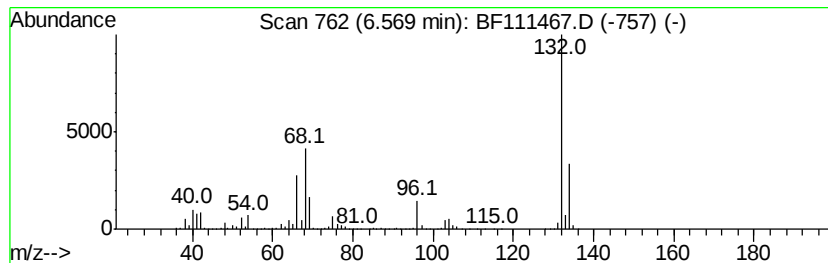
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Peak Number 2 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	97.85 ng	4656090	1,4-Dichlorobenzene-d4	6.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
3		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
4		Xenon	132	Xe	007440-63-3	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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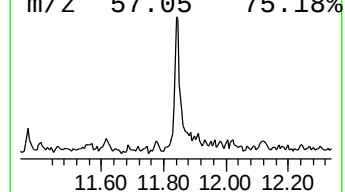
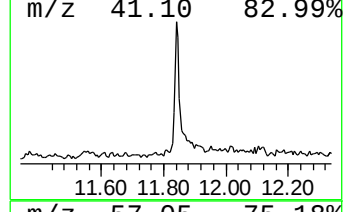
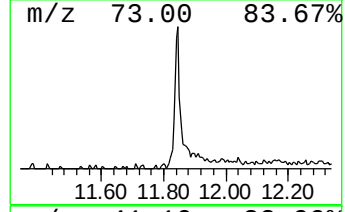
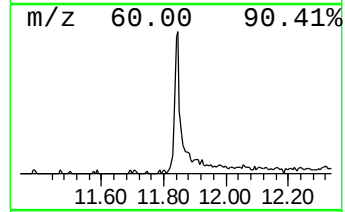
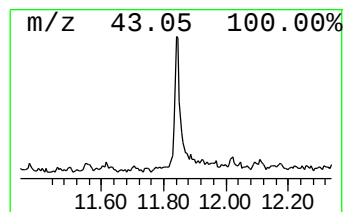
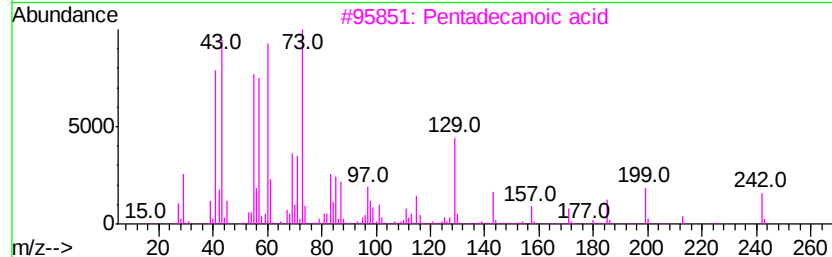
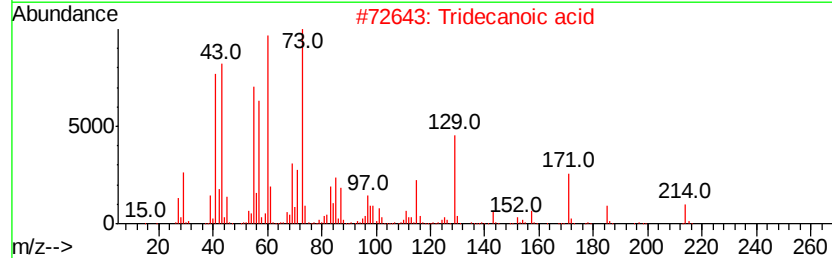
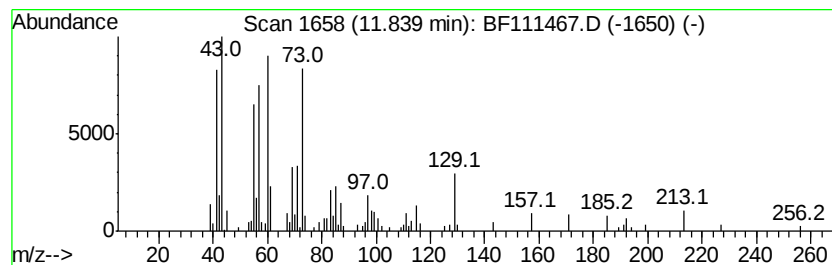
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.84	4.76 ng	257939	Phenanthrene-d10	11.31

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tridecanoic acid	214	C13H26O2	000638-53-9	95
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5		Undecanoic acid	186	C11H22O2	000112-37-8	53



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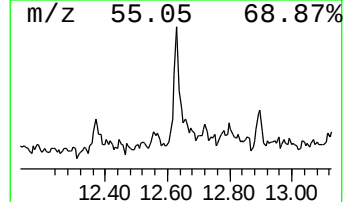
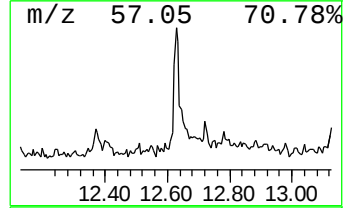
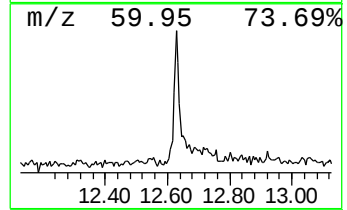
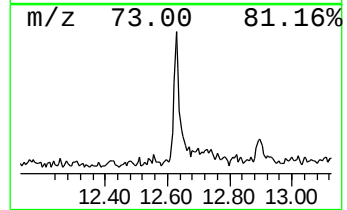
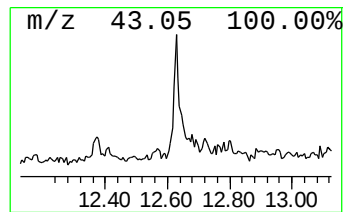
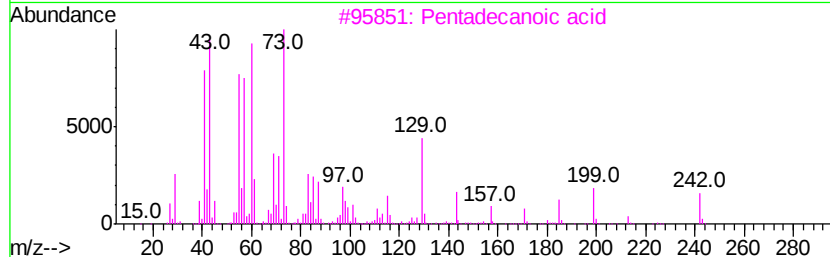
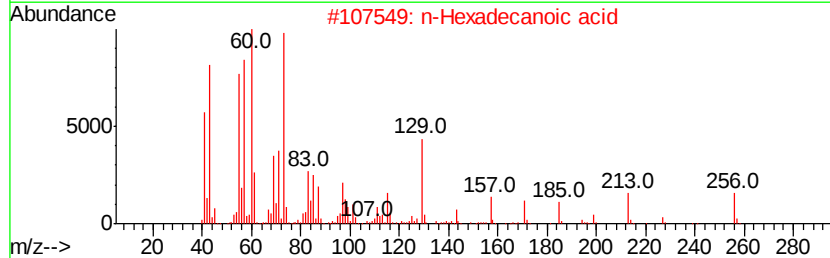
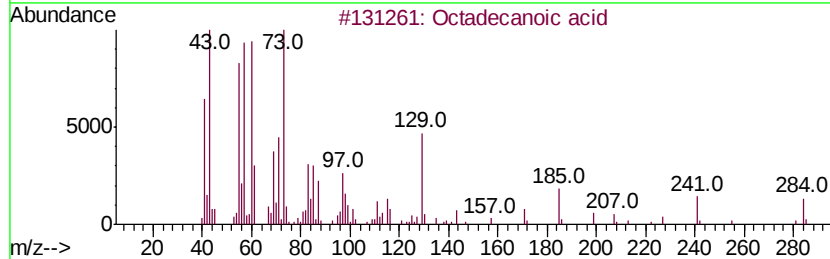
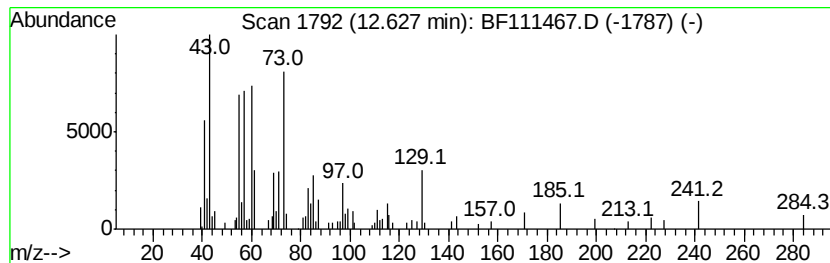
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Peak Number 5 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.63	2.96 ng	160418	Phenanthrene-d10	11.31

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	95
2		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	68
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	64
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5		Tridecanoic acid	214	C13H26O2	000638-53-9	58



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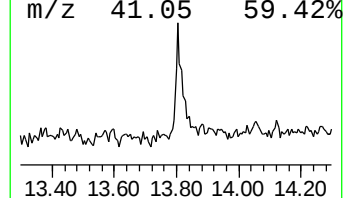
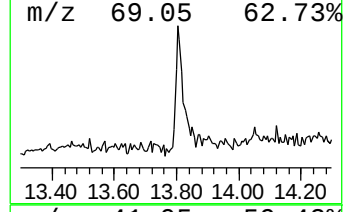
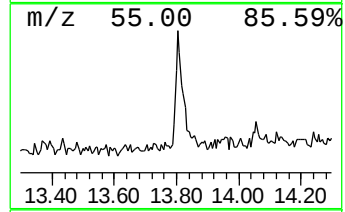
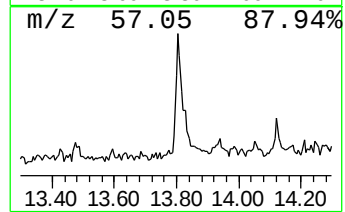
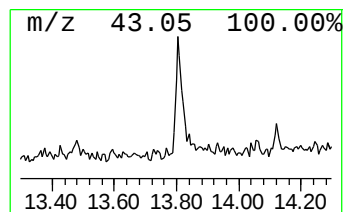
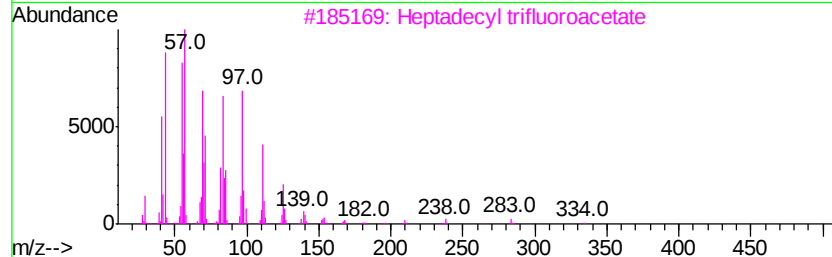
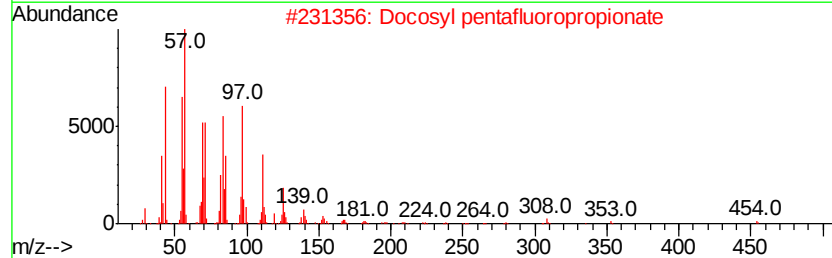
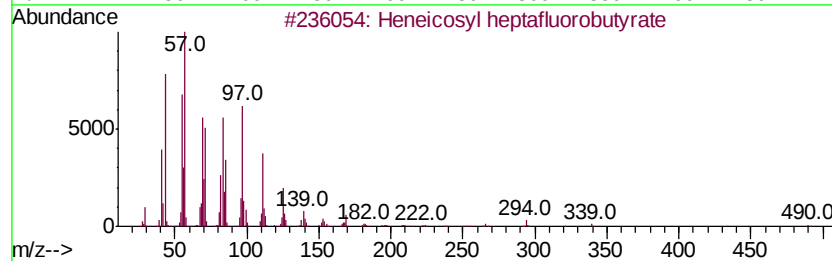
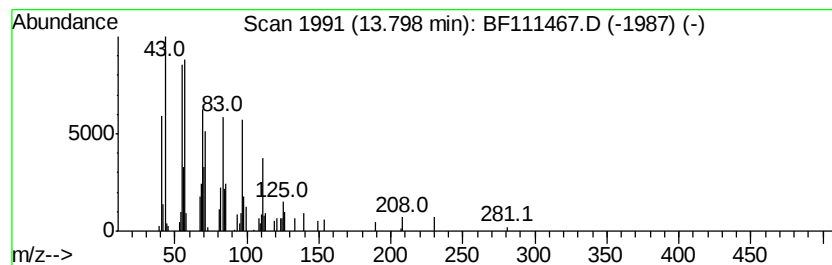
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Peak Number 6 Heneicosyl heptafluorobutyrate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.80	4.21 ng	182221	Chrysene-d12		13.94	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	87
2		Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	87
3		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	87
4		Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	83
5		Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	83



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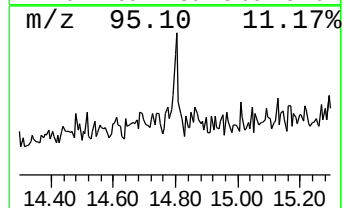
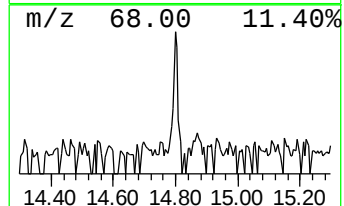
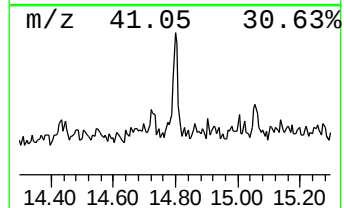
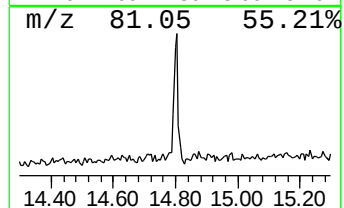
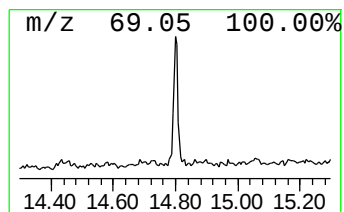
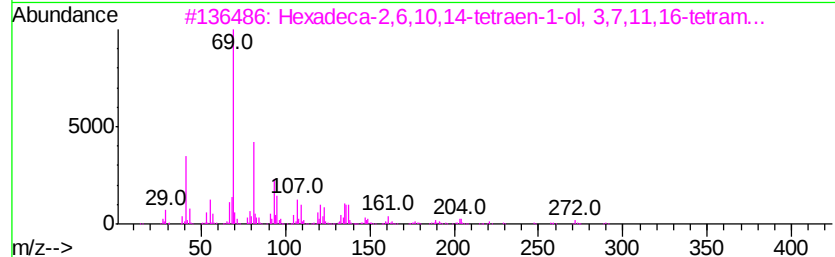
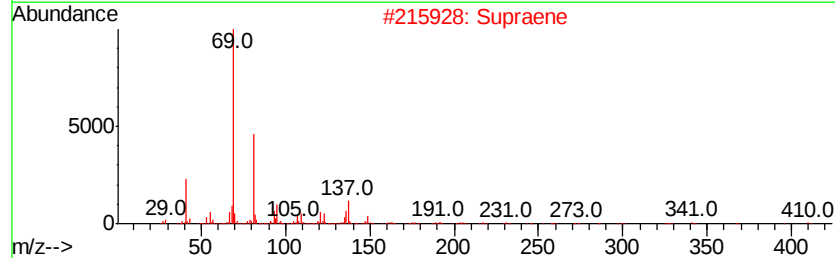
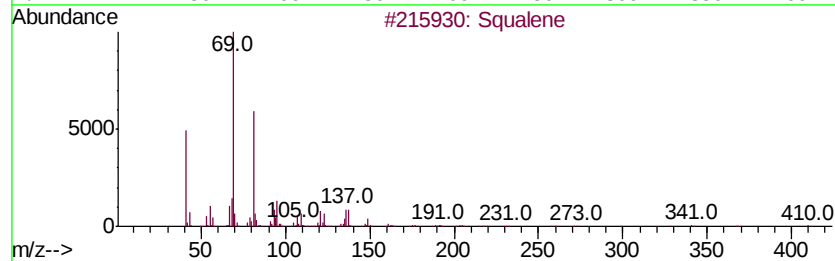
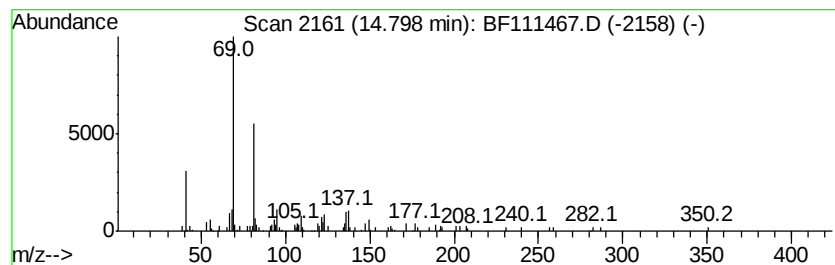
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Squalene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.80	2.05 ng	80484	Perylene-d12	15.39

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		Hexadeca-2,6,10,14-tetraen-1-ol,...	290	C20H34O	007614-21-3	80
4		1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	72
5		trans-Farnesol	222	C15H26O	000106-28-5	72



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF121518\
Data File : BF111467.D
Acq On : 15 Dec 2018 14:35
Operator : JU/SJ
Sample : J6322-19
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SUP-5A-C-1-120718

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121418.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...	5.01	5.1 ng		243140	1	6.79	951693	20.0
unknown6.57	6.57	97.8 ng		4656090	1	6.79	951693	20.0
n-Hexadecanoic acid	11.84	4.8 ng		257939	4	11.31	1084600	20.0
Octadecanoic acid	12.63	3.0 ng		160418	4	11.31	1084600	20.0
Heneicosyl heptaf...	13.80	4.2 ng		182221	5	13.94	866330	20.0
Squalene	14.80	2.0 ng		80484	6	15.39	783869	20.0