

Data Path : U:\HPCHEM1\BNA F\DATA\BF011118\
 Data File : BF102039.D
 Acq On : 12 Jan 2018 00:34
 Operator : SJ/JU
 Sample : J1082-02
 Misc :
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 EP-07

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:\HPCHEM1\BNA_F\METHODS\8270-BF010918.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	4.945	481	486	496	rVB	327703	519936	8.29%	0.939%
2	5.339	547	553	556	rBV	4986091	6100396	97.32%	11.012%
3	6.363	720	727	731	rBV	4590712	6268274	100.00%	11.315%
4	6.498	744	750	753	rBV	5500608	5920528	94.45%	10.687%
5	6.728	785	789	792	rVB	1555970	1357960	21.66%	2.451%
6	6.881	810	815	819	rBV	4518043	4626923	73.81%	8.352%
7	7.292	879	885	888	rBV	3551336	4013139	64.02%	7.244%
8	7.375	893	899	902	rVV	102593	122933	1.96%	0.222%
9	8.004	1002	1006	1009	rBV	2033522	1818502	29.01%	3.283%
10	8.028	1009	1010	1013	rVB	141786	68857	1.10%	0.124%
11	9.086	1184	1190	1193	rBV	5629688	6112615	97.52%	11.034%
12	9.480	1252	1257	1260	rBV	976263	778229	12.42%	1.405%
13	9.692	1291	1293	1297	rVB	181236	155834	2.49%	0.281%
14	9.757	1300	1304	1308	rVB	1927362	1767690	28.20%	3.191%
15	10.192	1376	1378	1381	rVB	221876	176364	2.81%	0.318%
16	10.416	1410	1416	1418	rBV	57837	75157	1.20%	0.136%
17	10.551	1433	1439	1442	rBV	3008943	3243574	51.75%	5.855%
18	10.669	1456	1459	1468	rVB	173730	205816	3.28%	0.372%
19	11.116	1532	1535	1537	rBV	126427	104968	1.67%	0.189%
20	11.239	1552	1556	1559	rBV	1858473	1621375	25.87%	2.927%
21	11.774	1644	1647	1657	rBV	292065	295387	4.71%	0.533%
22	12.727	1807	1809	1814	rVB	75667	67343	1.07%	0.122%
23	12.827	1821	1826	1830	rBV	3998165	4408009	70.32%	7.957%
24	13.721	1974	1978	1990	rBV	809791	731552	11.67%	1.321%
25	13.868	1998	2003	2007	rBV2	3200517	3223799	51.43%	5.819%
26	14.357	2082	2086	2096	rBV3	60936	80210	1.28%	0.145%
27	14.721	2145	2148	2153	rVB	152499	138817	2.21%	0.251%
28	15.292	2239	2245	2250	rBV	889923	1111197	17.73%	2.006%
29	15.786	2325	2329	2334	rBV	101737	143679	2.29%	0.259%
30	17.209	2566	2571	2580	rVB6	65951	139392	2.22%	0.252%

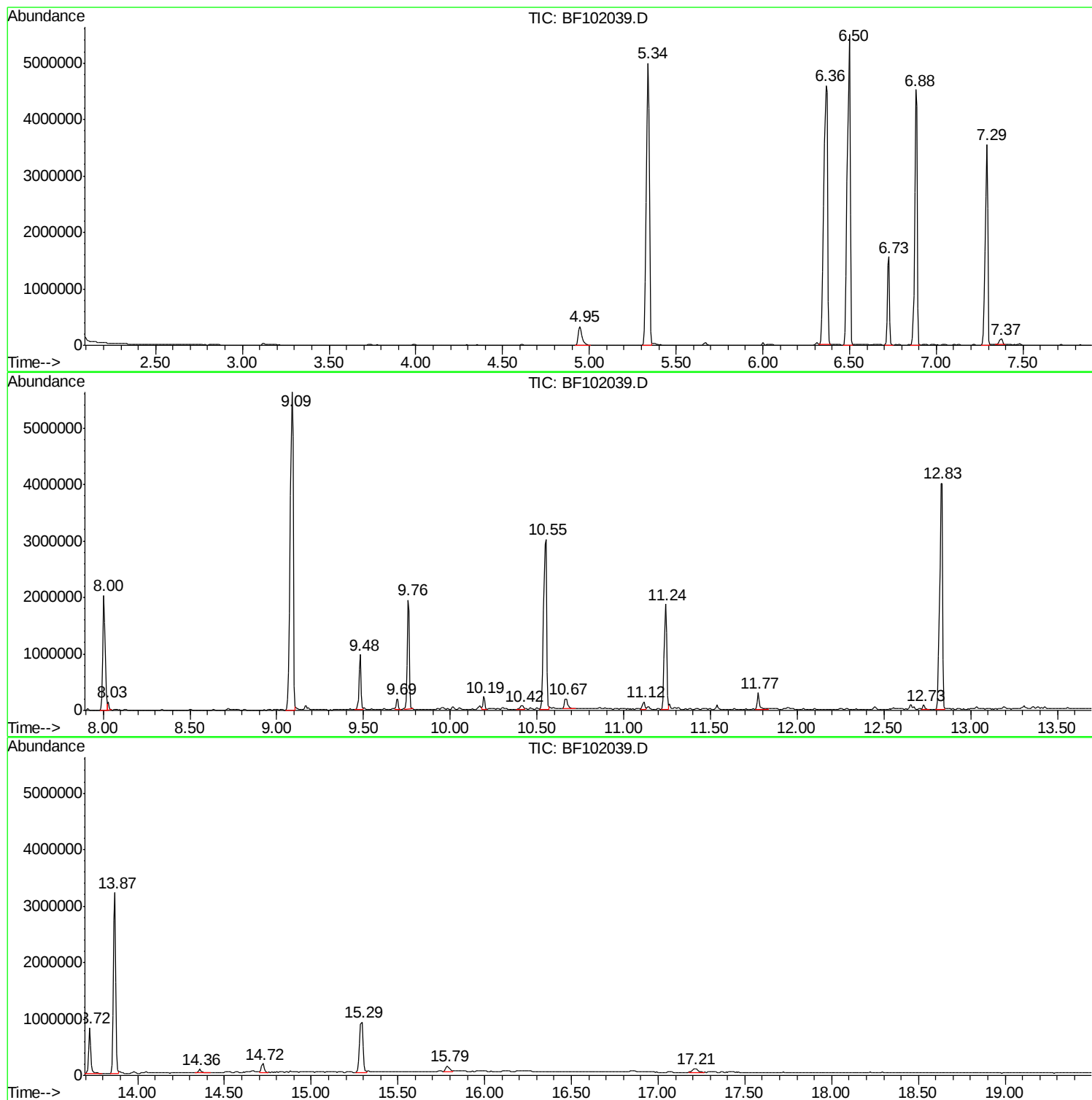
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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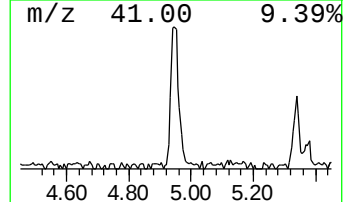
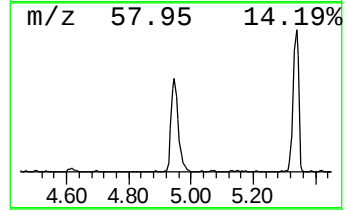
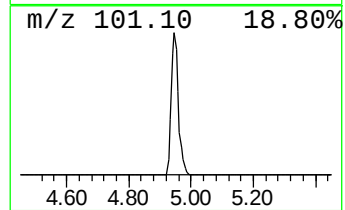
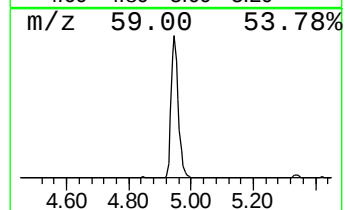
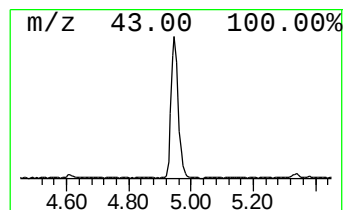
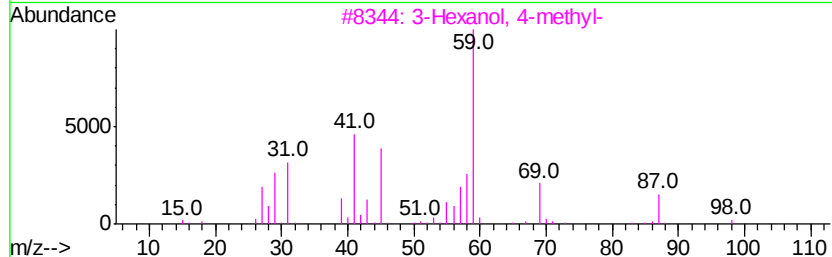
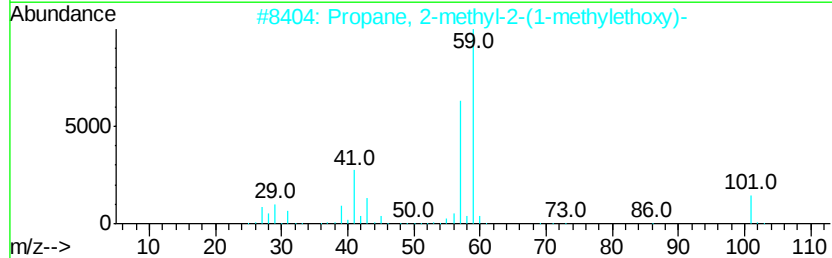
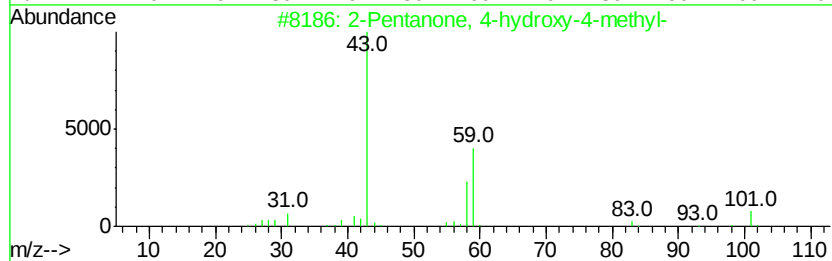
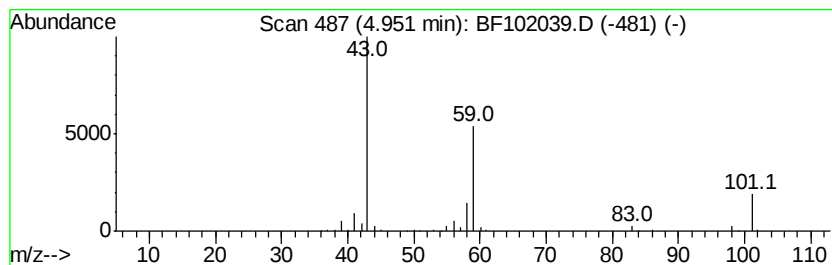
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.95	7.66 ng	519936	1,4-Dichlorobenzene-d4	6.73

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16



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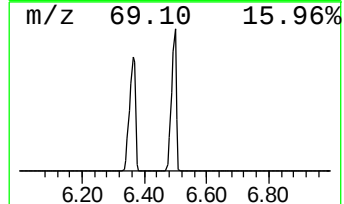
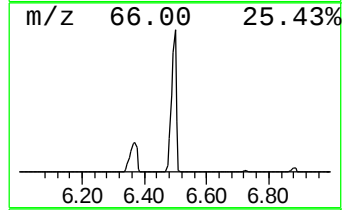
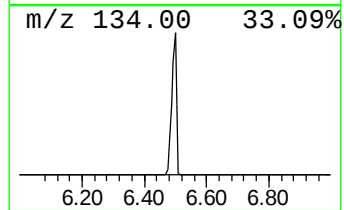
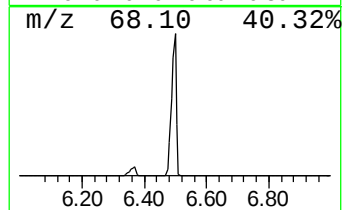
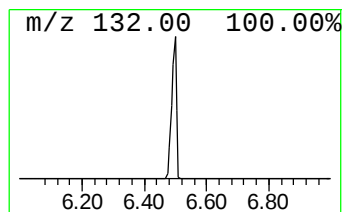
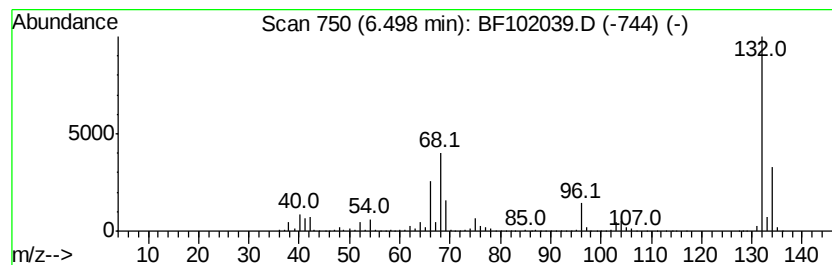
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	87.20 ng	5920530	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	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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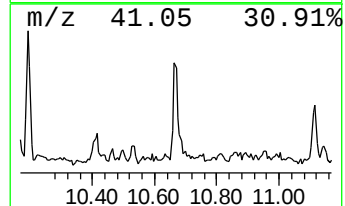
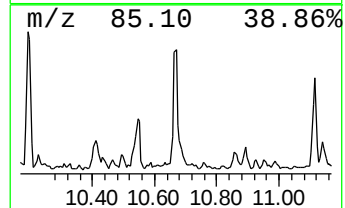
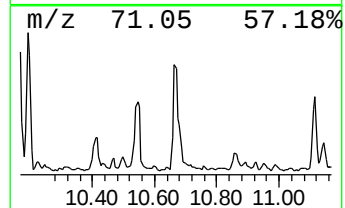
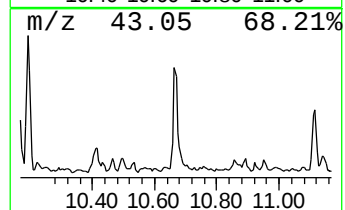
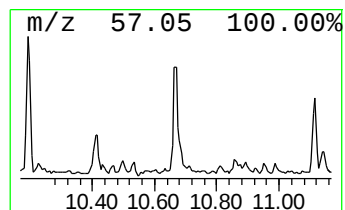
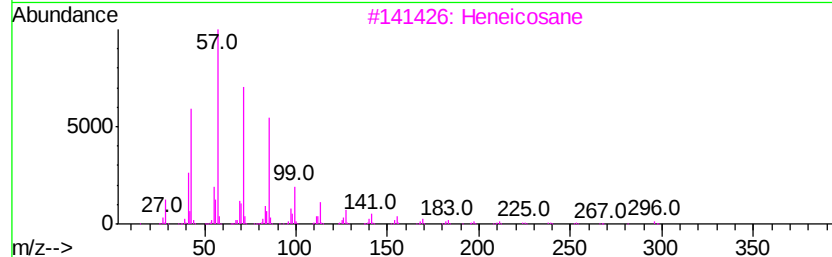
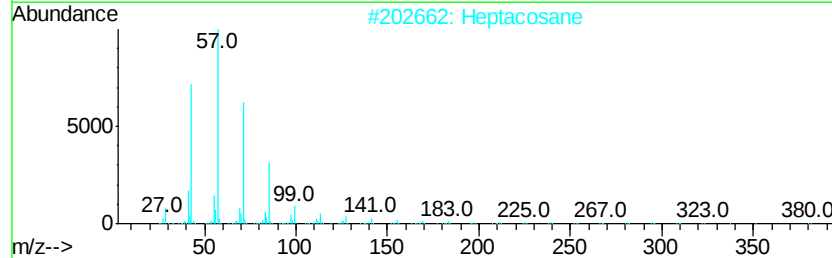
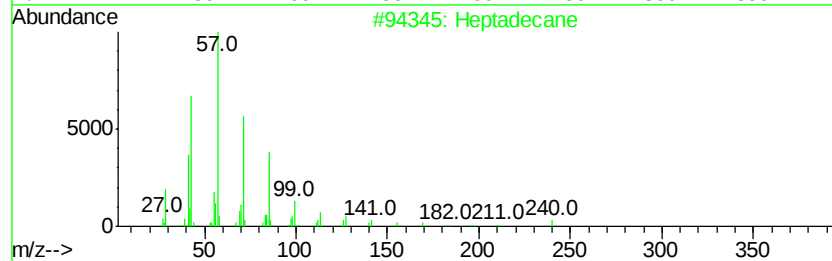
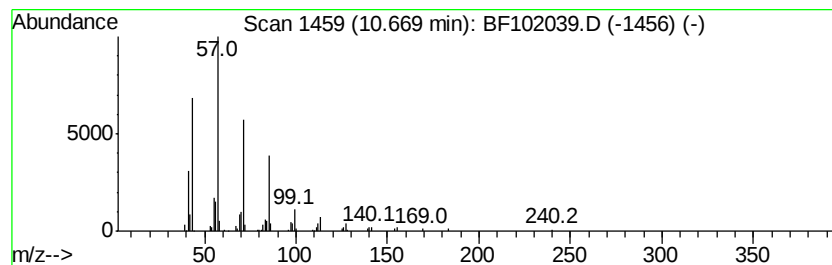
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Peak Number 4 Heptadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.67	2.54 ng	205816	Phenanthrene-d10	11.24

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane		240	C17H36	000629-78-7	97
2	Heptacosane		380	C27H56	000593-49-7	91
3	Heneicosane		296	C21H44	000629-94-7	90
4	Hexadecane		226	C16H34	000544-76-3	90
5	Eicosane, 10-methyl-		296	C21H44	054833-23-7	87



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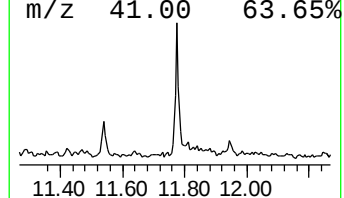
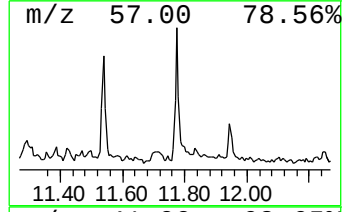
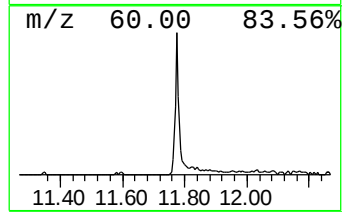
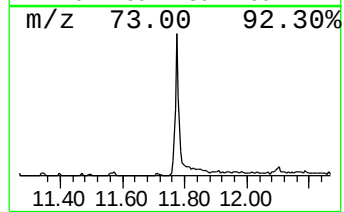
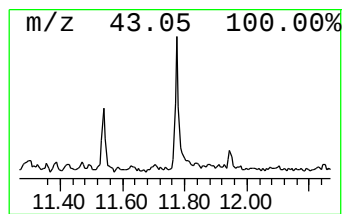
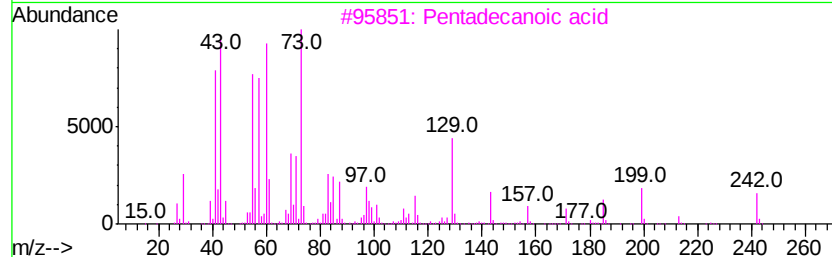
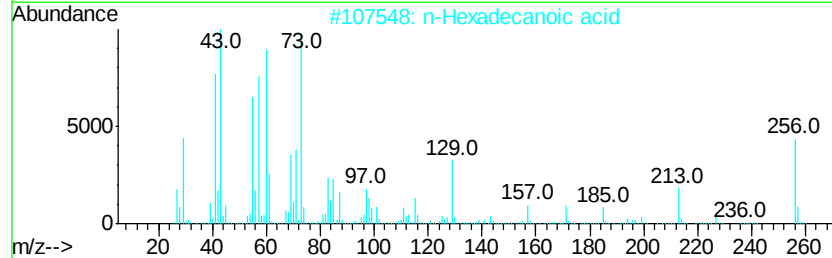
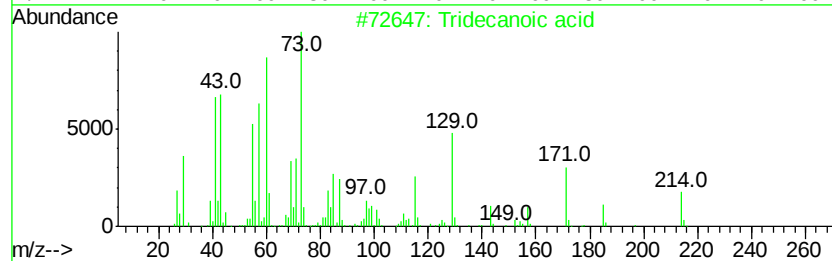
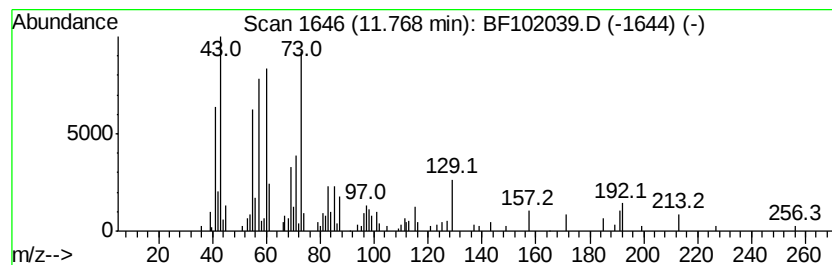
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Peak Number 5 Tridecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.77	3.64 ng	295387	Phenanthrene-d10	11.24

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tridecanoic acid	214	C13H26O2	000638-53-9	95
2		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	86
5		Dodecane	170	C12H26	000112-40-3	11



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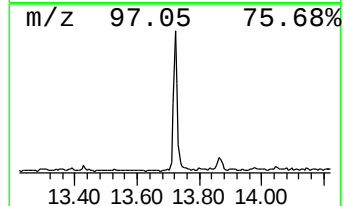
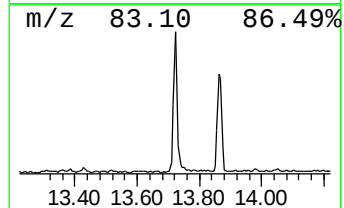
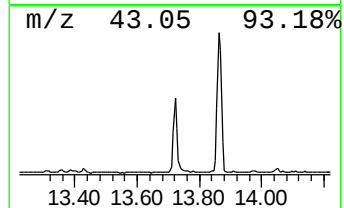
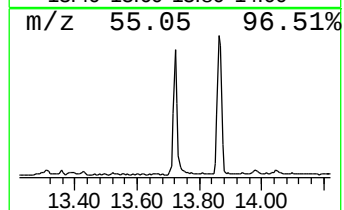
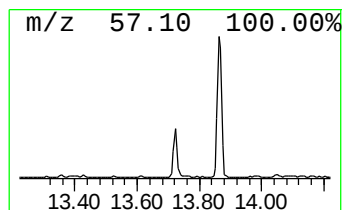
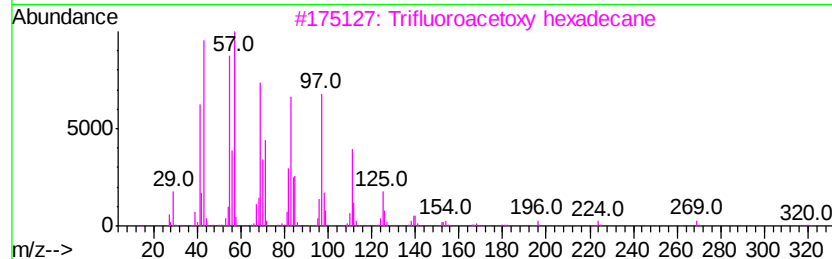
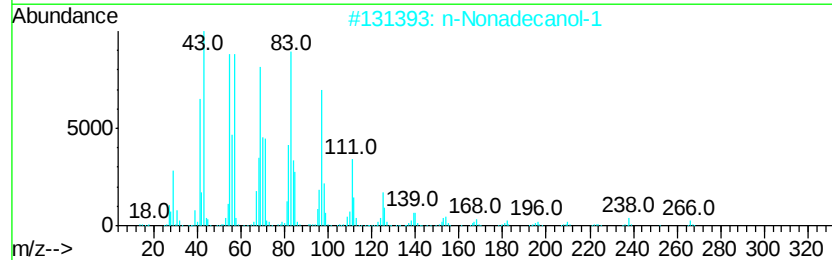
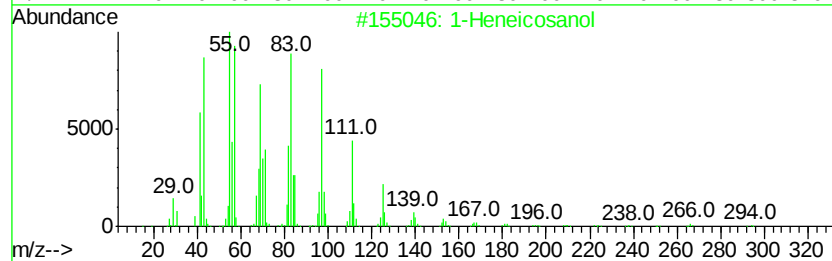
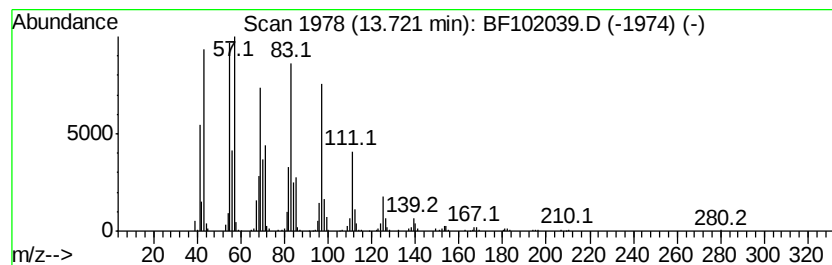
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Peak Number 6 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.72	4.54 ng	731552	Chrysene-d12	13.87	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
4	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93
5	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	93



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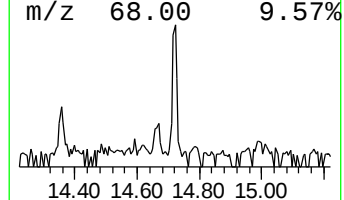
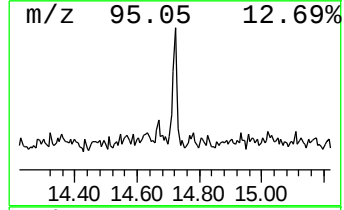
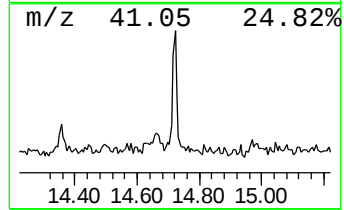
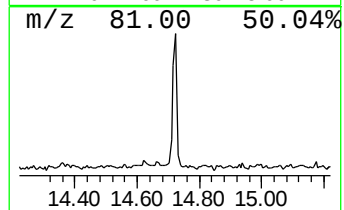
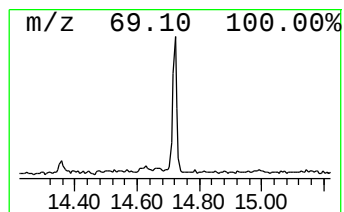
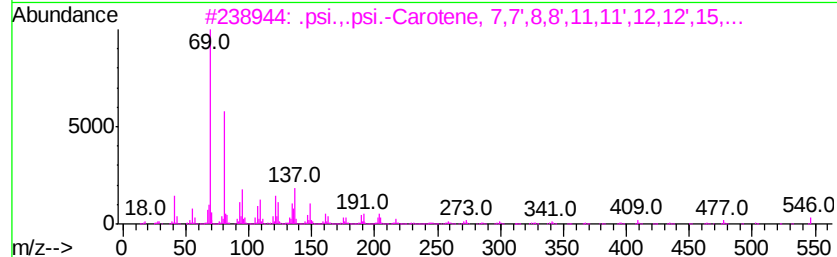
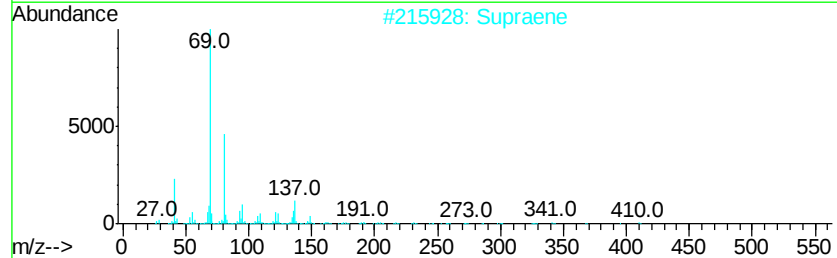
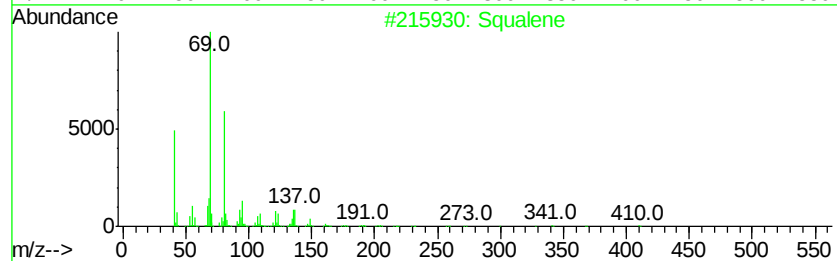
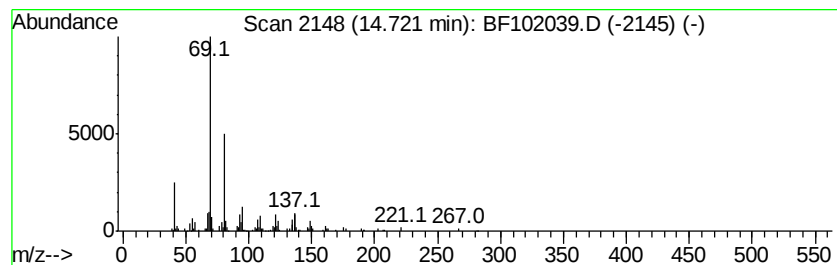
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Squalene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.72	2.50 ng	138817	Perylene-d12	15.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	91
2		Supraene	410	C30H50	007683-64-9	87
3		.psi.,.psi.-Carotene, 7,7',8,8',....	547	C40H66	000502-62-5	83
4		7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	80
5		(.+/-)-Lavandulol, pentafluorop...	300	C13H17F5O2	1000352-63-1	72



Data Path : U:\HPCHEM1\BNA_F\DATA\BF011118\
Data File : BF102039.D
Acq On : 12 Jan 2018 00:34
Operator : SJ/JU
Sample : J1082-02
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EP-07

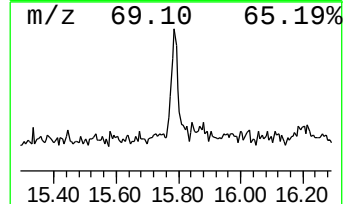
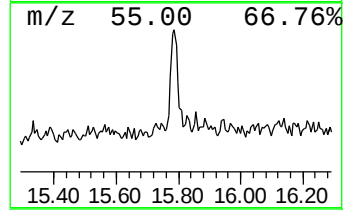
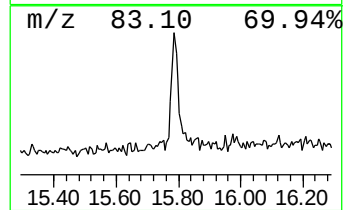
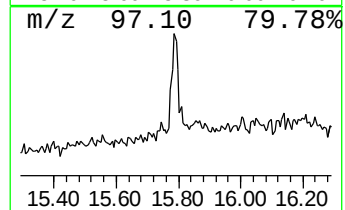
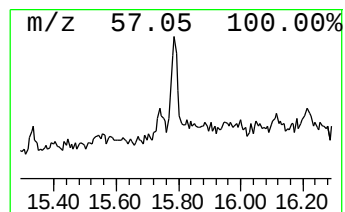
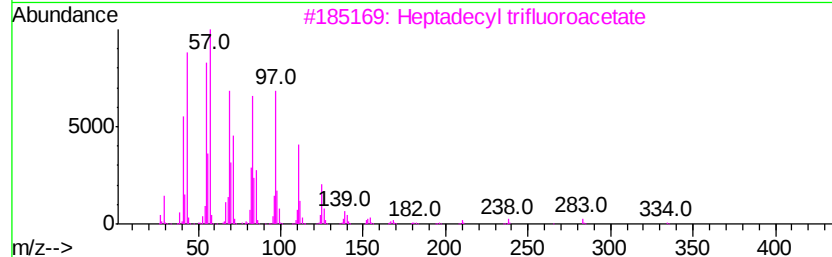
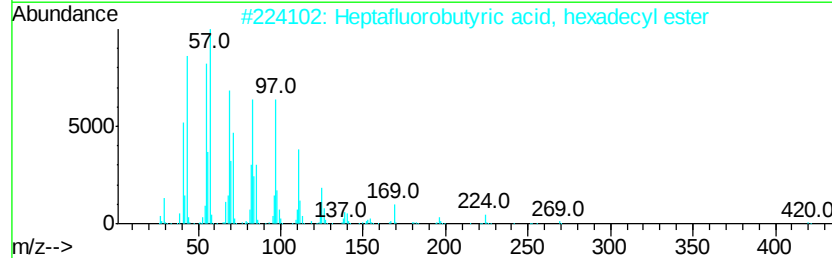
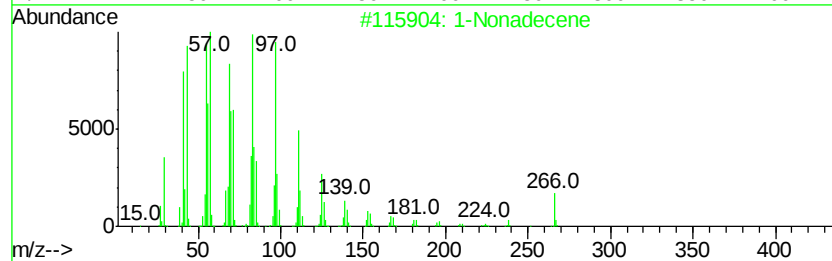
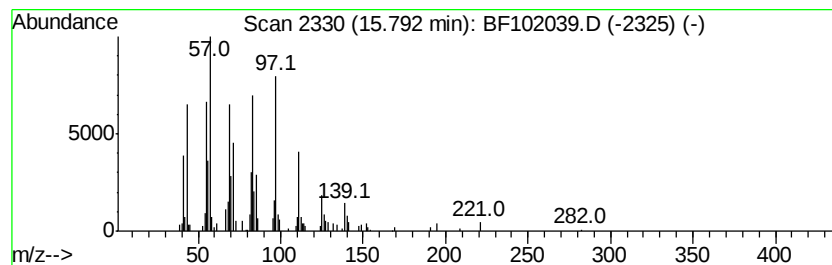
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1-Nonadecene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.79	2.59 ng	143679	Perylene-d12	15.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Nonadecene	266	C19H38	018435-45-5	93
2		Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	91
3		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	91
4		Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	91
5		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91



Data Path : U:\HPCHEM1\BNA F\DATA\BF011118\
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Acq On : 12 Jan 2018 00:34
Operator : SJ/JU
Sample : J1082-02
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EP-07

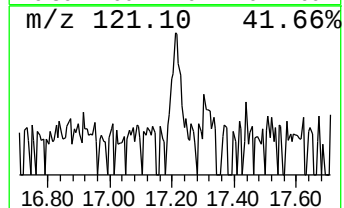
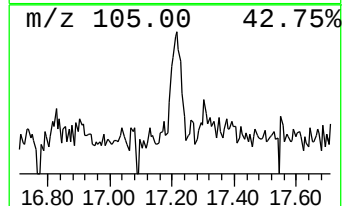
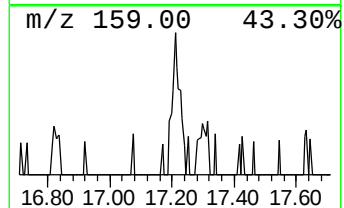
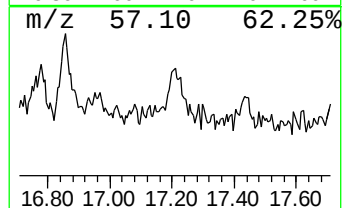
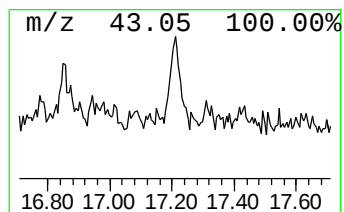
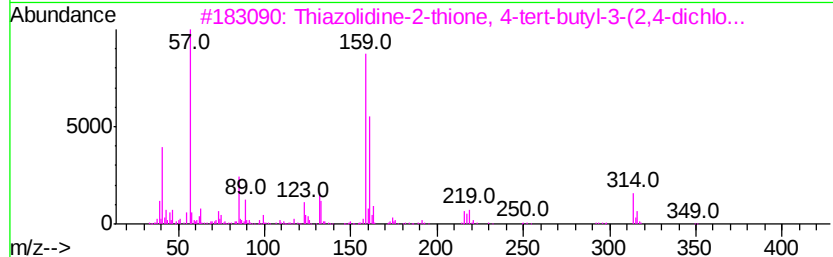
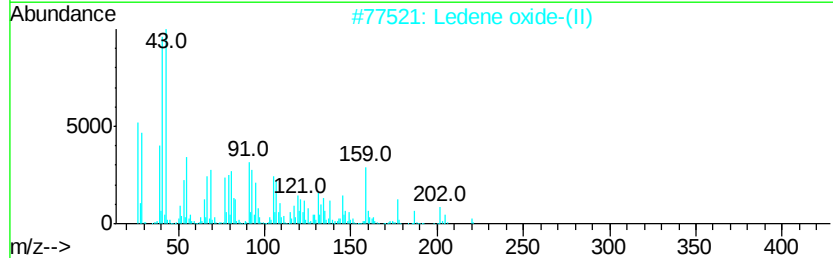
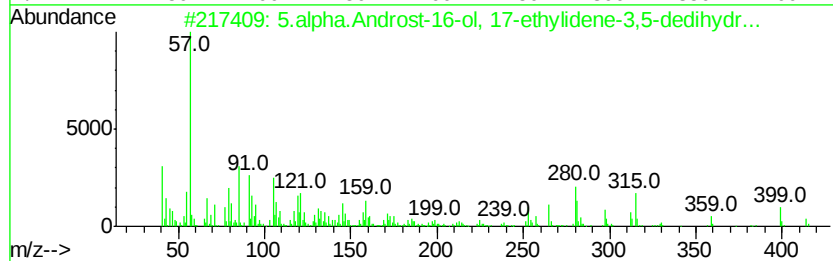
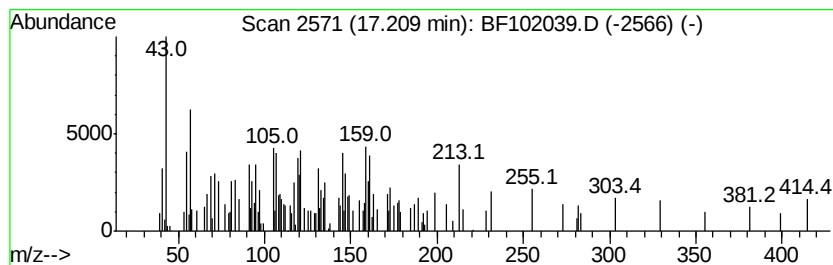
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown17.21 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.21	2.51 ng	139392	Perylene-d12	15.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5.alpha.Androst-16-ol, 17-ethyl...	414	C27H42O3	1000124-58-6	38
2		Ledene oxide-(II)	220	C15H24O	1000159-36-7	25
3		Thiazolidine-2-thione, 4-tert-bu...	349	C14H17Cl2NOS2	1000264-76-1	22
4		2,3-Dichlorobenzyl alcohol, neop...	246	C12H16Cl2O	1000375-30-1	22
5		Pregn-4-ene-3,20-dione, 17-(acet...	386	C24H34O4	002504-36-1	17



Data Path : U:\HPCHEM1\BNA_F\DATA\BF011118\
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Sample : J1082-02
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EP-07

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.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...	4.95	7.7	ng	519936	1	6.73	1357960	20.0
unknown6.50	6.50	87.2	ng	5920530	1	6.73	1357960	20.0
Heptadecane	10.67	2.5	ng	205816	4	11.24	1621380	20.0
Tridecanoic acid	11.77	3.6	ng	295387	4	11.24	1621380	20.0
1-Heneicosanol	13.72	4.5	ng	731552	5	13.87	3223800	20.0
Squalene	14.72	2.5	ng	138817	6	15.29	1111200	20.0
1-Nonadecene	15.79	2.6	ng	143679	6	15.29	1111200	20.0
unknown17.21	17.21	2.5	ng	139392	6	15.29	1111200	20.0