

Data Path : Z:\HPCHEM1\BNA F\DATA\BF041118\
 Data File : BF104437.D
 Acq On : 11 Apr 2018 14:49
 Operator : JU/SJ
 Sample : J2310-05 2X
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 P004-S004-0001-01

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-BF040618.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	5.004	493	496	502	rVB	54341	59531	3.80%	0.375%
2	5.416	561	566	569	rBV	1450075	1313644	83.96%	8.277%
3	6.434	734	739	742	rBV	1563737	1336873	85.44%	8.424%
4	6.575	759	763	766	rBV	1643979	1393008	89.03%	8.777%
5	6.804	799	802	806	rBV	869090	762490	48.73%	4.804%
6	6.963	825	829	832	rBV	1276141	1067544	68.23%	6.727%
7	7.369	893	898	901	rBV	966974	803779	51.37%	5.065%
8	8.092	1016	1021	1024	rBV	1117085	981855	62.75%	6.187%
9	9.163	1199	1203	1207	rBV	1820964	1564623	100.00%	9.859%
10	9.557	1267	1270	1274	rBV	87118	72919	4.66%	0.459%
11	9.774	1302	1307	1310	rBV	35918	30839	1.97%	0.194%
12	9.845	1315	1319	1323	rBV	1148740	944090	60.34%	5.949%
13	10.274	1389	1392	1395	rVB	51508	39542	2.53%	0.249%
14	10.633	1449	1453	1457	rBV	938535	766866	49.01%	4.832%
15	10.751	1469	1473	1477	rBV	63980	63793	4.08%	0.402%
16	11.198	1546	1549	1552	rBV	41428	35219	2.25%	0.222%
17	11.274	1560	1562	1567	rBV3	19714	23008	1.47%	0.145%
18	11.333	1568	1572	1575	rBV	923445	771635	49.32%	4.862%
19	11.498	1598	1600	1604	rVB	21949	20035	1.28%	0.126%
20	11.551	1604	1609	1615	rBV4	13930	21762	1.39%	0.137%
21	11.863	1658	1662	1666	rBV	127426	120414	7.70%	0.759%
22	12.033	1688	1691	1696	rVB4	17634	19726	1.26%	0.124%
23	12.474	1764	1766	1773	rVB	27822	24338	1.56%	0.153%
24	12.804	1819	1822	1826	rBV2	13124	18291	1.17%	0.115%
25	12.921	1838	1842	1846	rBV	1387337	1194379	76.34%	7.526%
26	13.786	1986	1989	1991	rBV	30800	27447	1.75%	0.173%
27	13.815	1991	1994	1998	rVV	184061	164649	10.52%	1.037%
28	13.980	2015	2022	2025	rBV	856979	831225	53.13%	5.238%
29	14.457	2101	2103	2108	rVB	42523	46801	2.99%	0.295%
30	14.509	2110	2112	2117	rVB4	38931	38027	2.43%	0.240%
31	14.745	2149	2152	2162	rVB	121759	151270	9.67%	0.953%
32	15.098	2210	2212	2215	rBV2	31469	33312	2.13%	0.210%
33	15.445	2267	2271	2276	rBV	464364	585327	37.41%	3.688%
34	15.962	2355	2359	2366	rVB5	57001	96246	6.15%	0.606%

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35	17.062	2542	2546	2556	rVB10	59632	139343	8.91%	0.878%
36	17.474	2612	2616	2626	rVB9	72487	168797	10.79%	1.064%
37	18.503	2787	2791	2804	rVB9	44576	137698	8.80%	0.868%

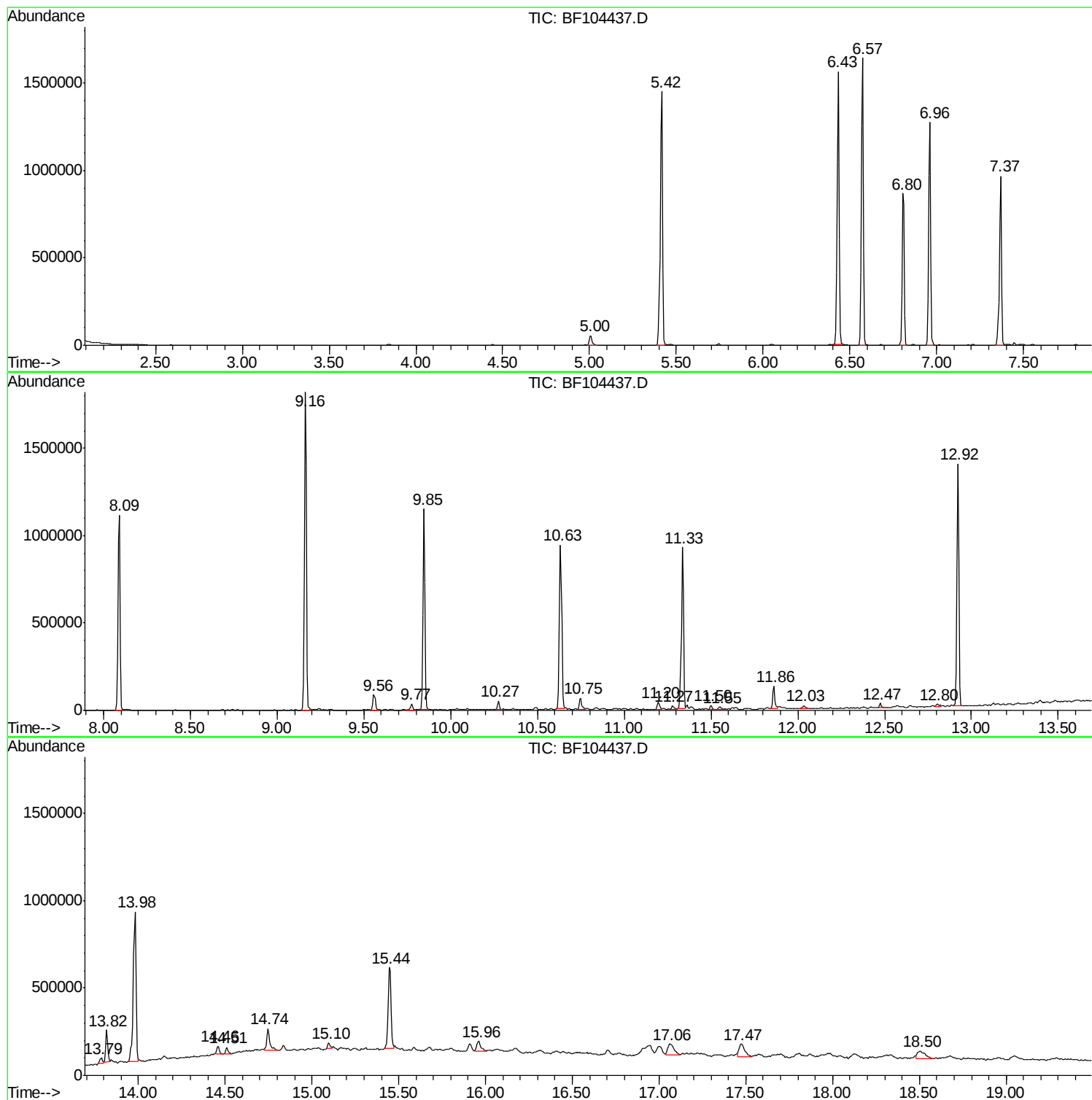
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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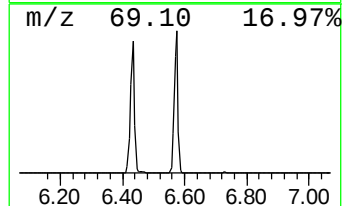
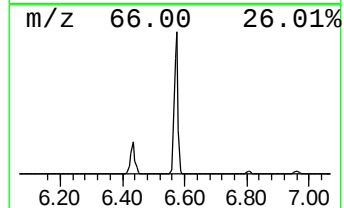
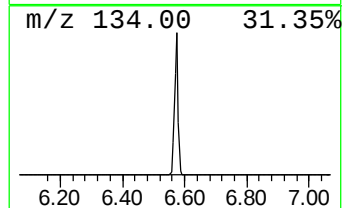
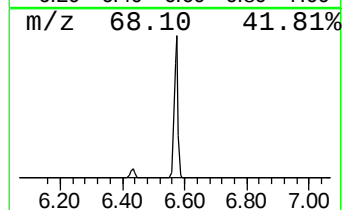
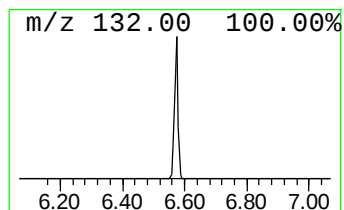
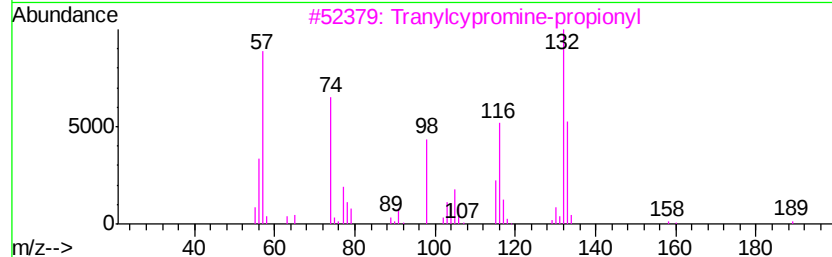
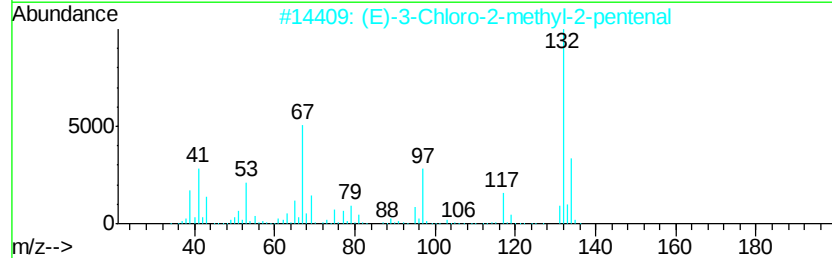
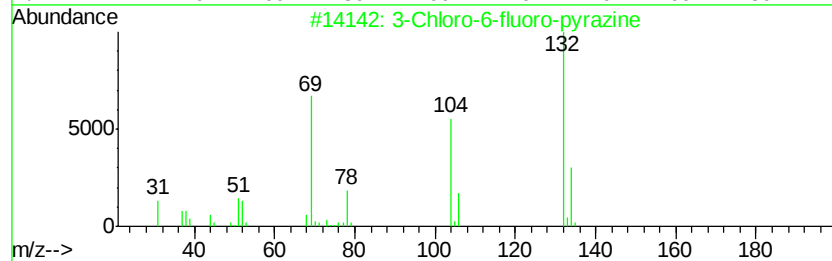
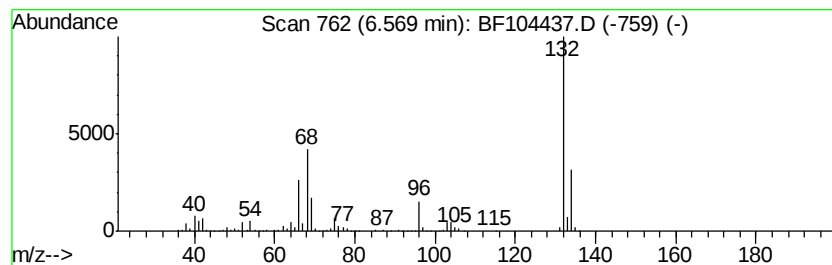
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	36.54 ng	1393010	1,4-Dichlorobenzene-d4	6.80

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	16
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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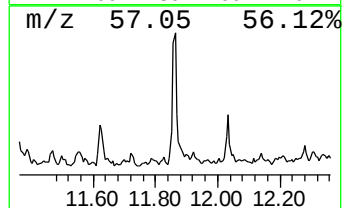
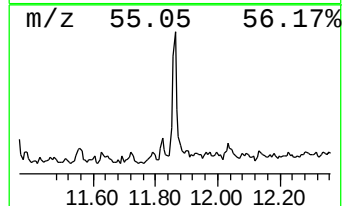
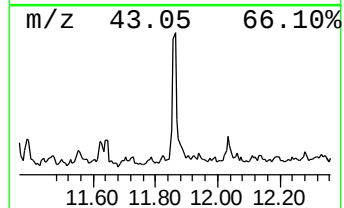
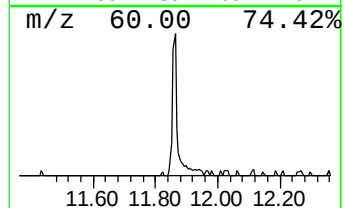
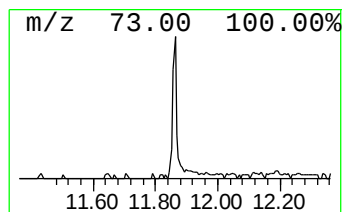
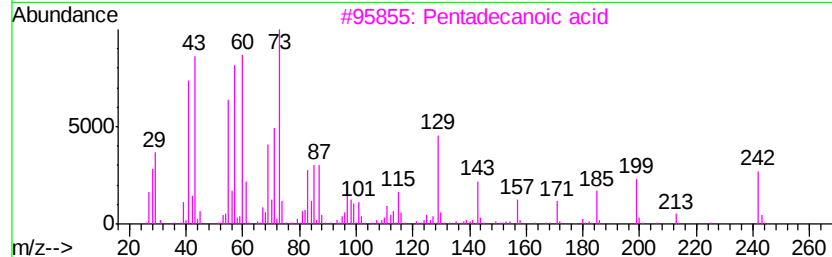
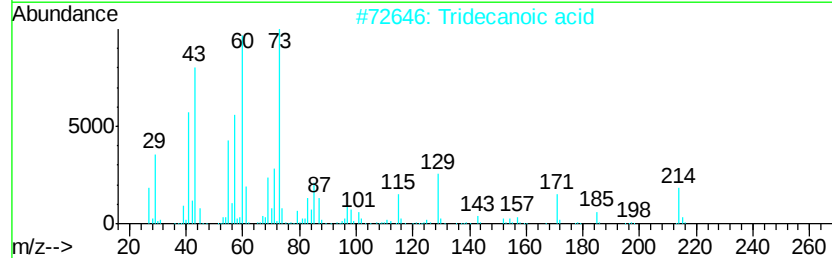
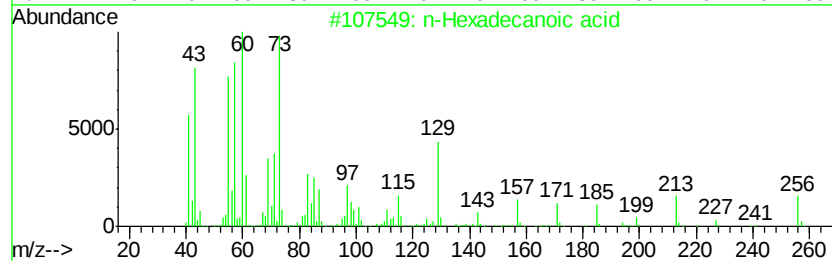
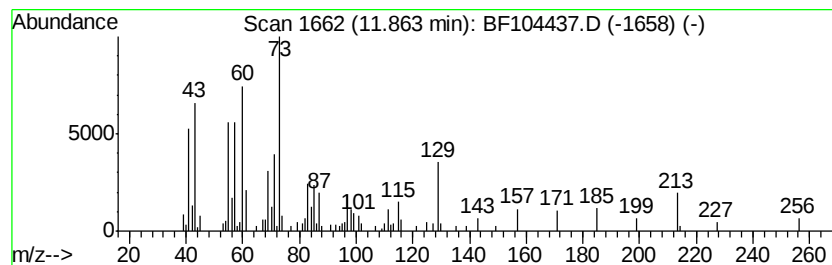
Instrument :
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.86	3.12 ng	120414	Phenanthrene-d10	11.33	
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	87
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	Oxalic acid, dodecyl propyl ester	300	C17H32O4	1000309-26-5	20



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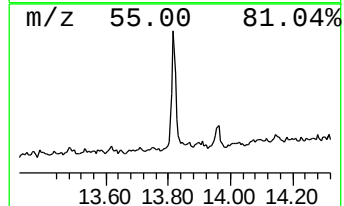
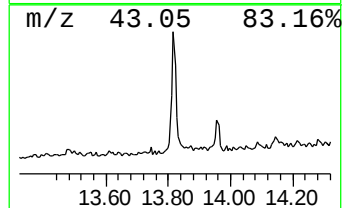
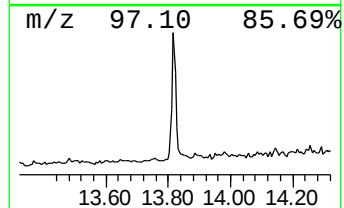
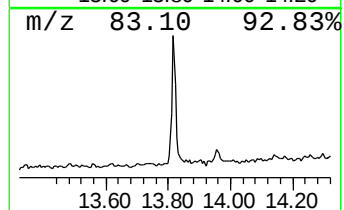
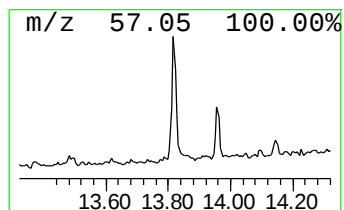
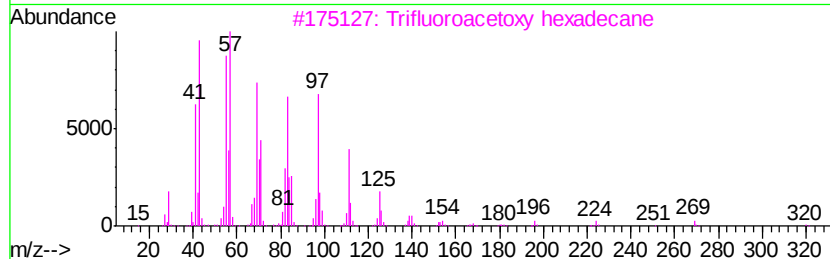
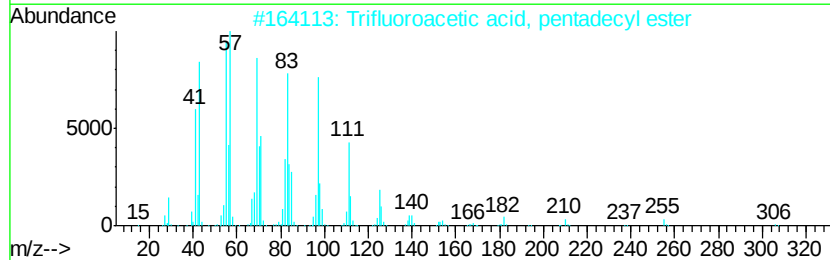
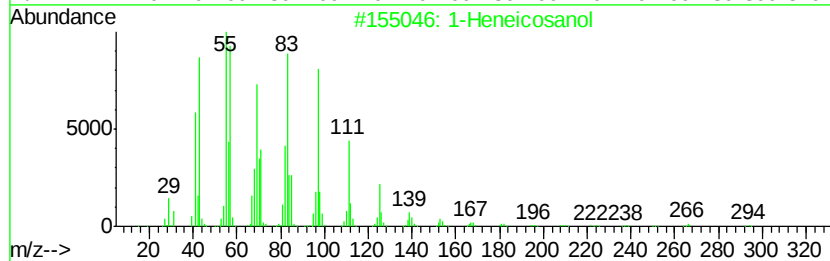
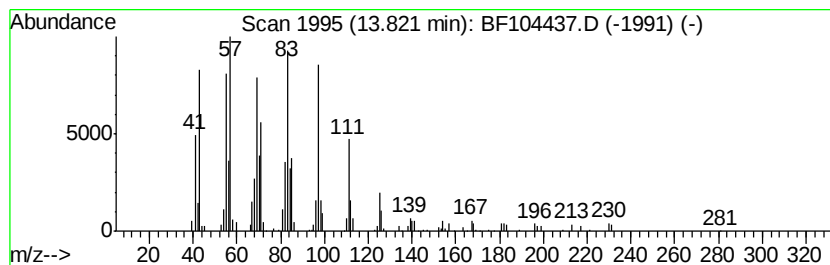
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Peak Number 4 1-Heneicosanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.82	3.96 ng	164649	Chrysene-d12	13.98

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Heneicosanol	312	C21H44O	015594-90-8	95
2		Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	93
3		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
4		Heptafluorobutyric acid, penta...	424	C19H31F7O2	959261-23-5	93
5		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	93



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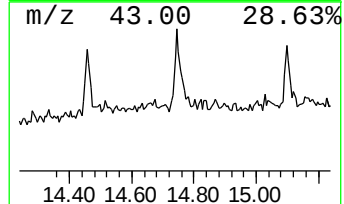
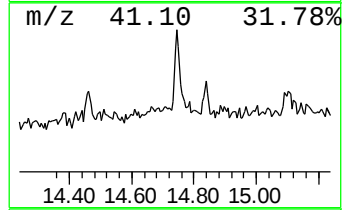
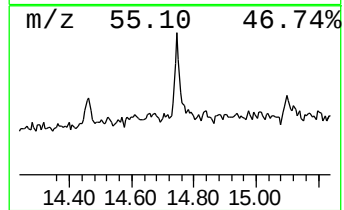
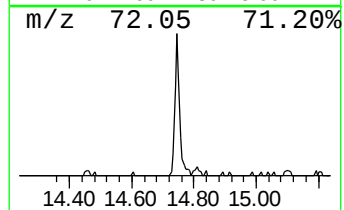
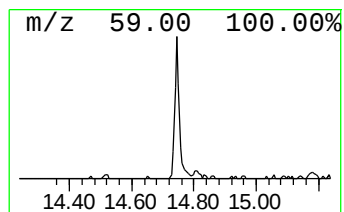
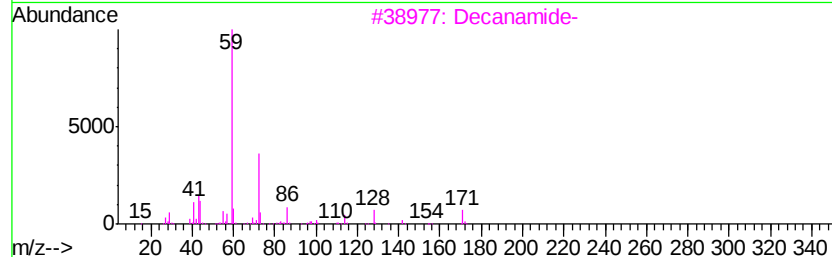
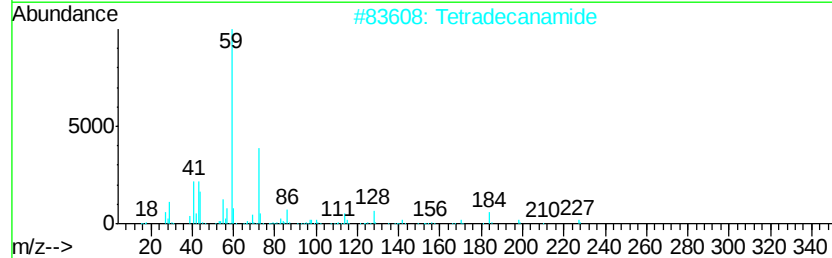
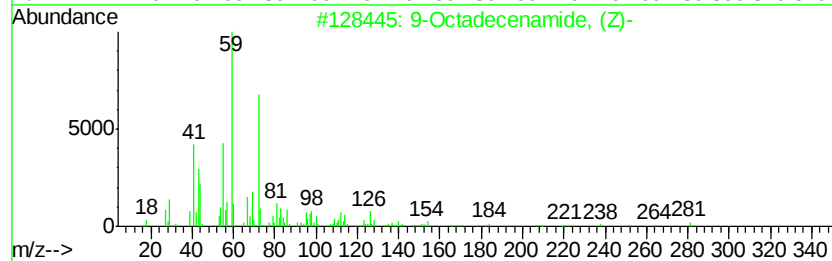
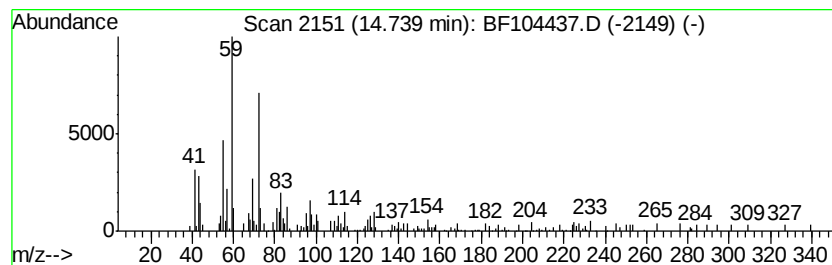
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Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.74	5.17 ng	151270	Perylene-d12	15.44

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	87
2		Tetradecanamide	227	C14H29NO	000638-58-4	68
3		Decanamide-	171	C10H21NO	002319-29-1	50
4		Octadecanamide	283	C18H37NO	000124-26-5	47
5		Silane, hexyl-	116	C6H16Si	001072-14-6	43



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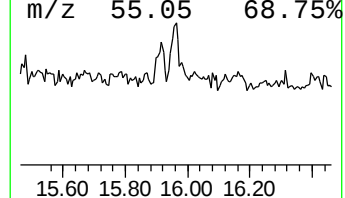
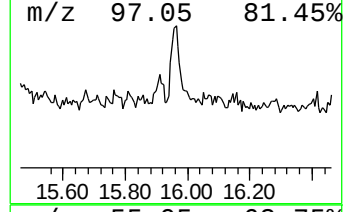
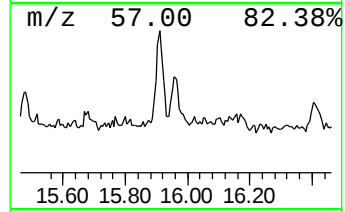
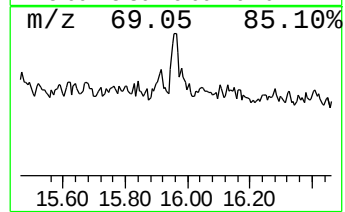
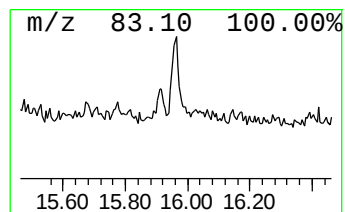
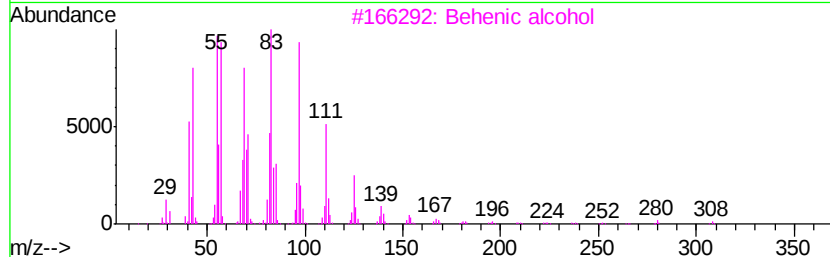
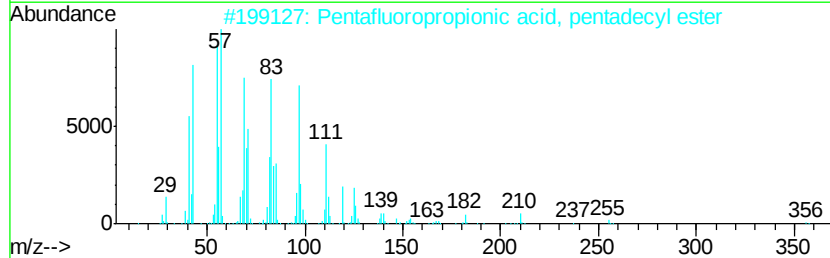
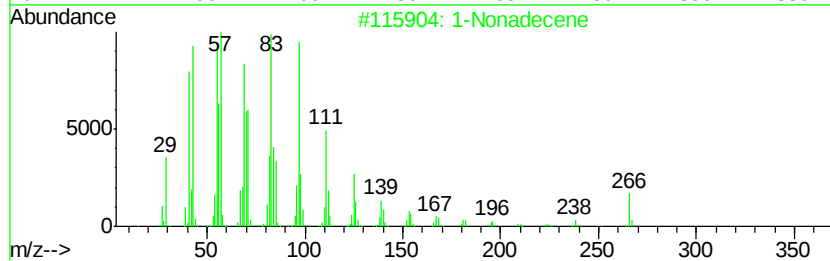
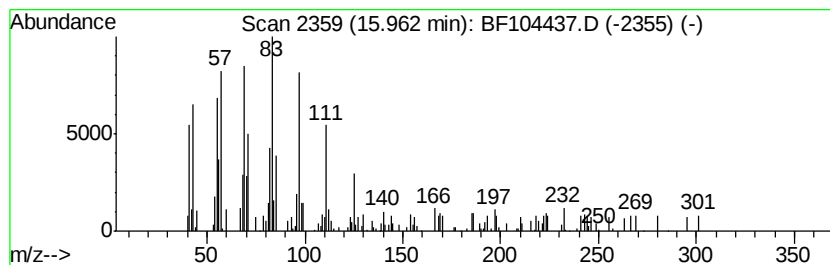
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Peak Number 6 1-Nonadecene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.96	3.29 ng	96246	Perylene-d12	15.44

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene		266	C19H38	018435-45-5	94
2	Pentafluoropropionic acid, penta...		374	C18H31F5O2	959092-08-1	90
3	Behenic alcohol		326	C22H46O	000661-19-8	83
4	Cyclohexadecane, 1,2-diethyl-		280	C20H40	1000155-85-3	81
5	Cyclohexadecane		224	C16H32	000295-65-8	81



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF041118\
Data File : BF104437.D
Acq On : 11 Apr 2018 14:49
Operator : JU/SJ
Sample : J2310-05 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P004-S004-0001-01

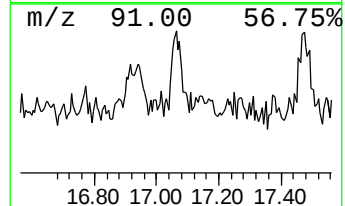
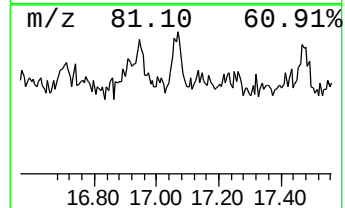
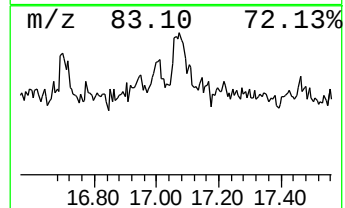
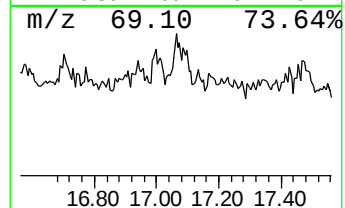
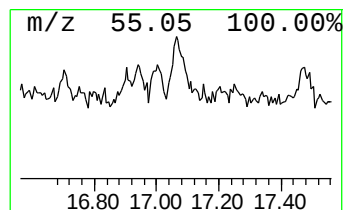
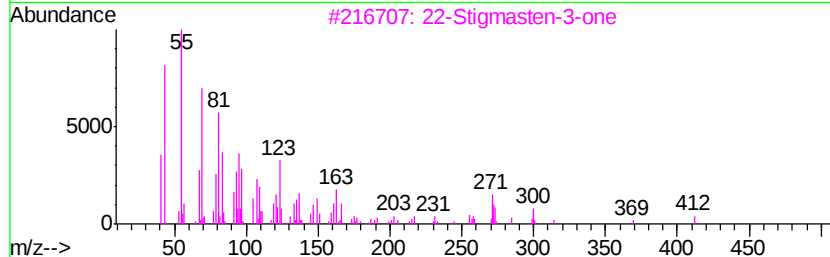
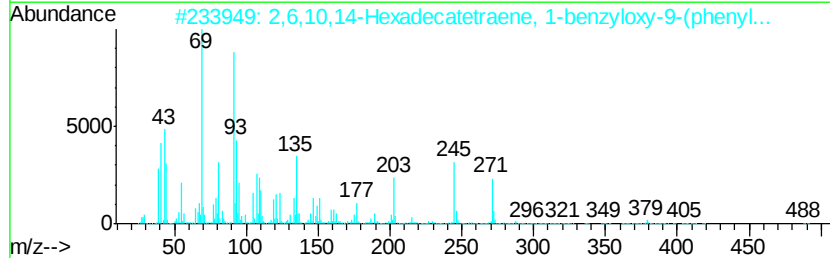
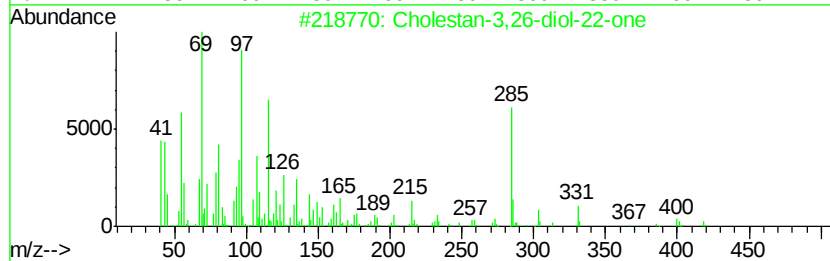
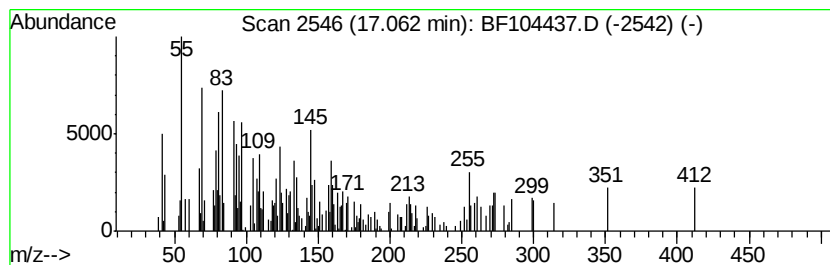
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown17.06 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.06	4.76 ng	139343	Perylene-d12	15.44

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cholestan-3,26-diol-22-one	418	C27H46O3	1000252-39-3	22
2		2,6,10,14-Hexadecatetraene, 1-be...	488	C33H44OS	1000194-30-4	14
3		22-Stigmasten-3-one	412	C29H48O	004736-95-2	12
4		Cyclohexanone, 2-(1-mercapto-1-m...	186	C10H18OS	033281-91-3	12
5		1,2-Benzendiol, 0-cyclopentaneca...	352	C15H13F5O4	1000330-09-8	12



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF041118\
Data File : BF104437.D
Acq On : 11 Apr 2018 14:49
Operator : JU/SJ
Sample : J2310-05 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

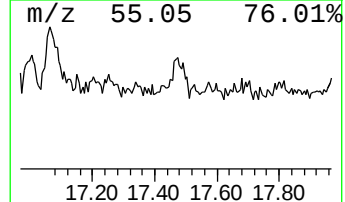
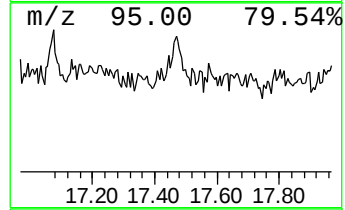
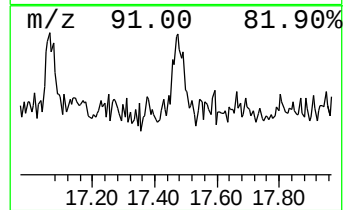
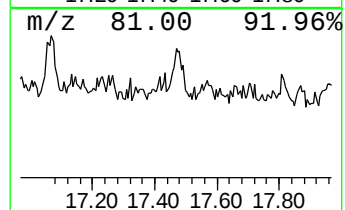
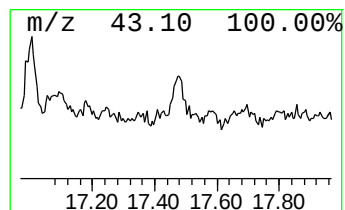
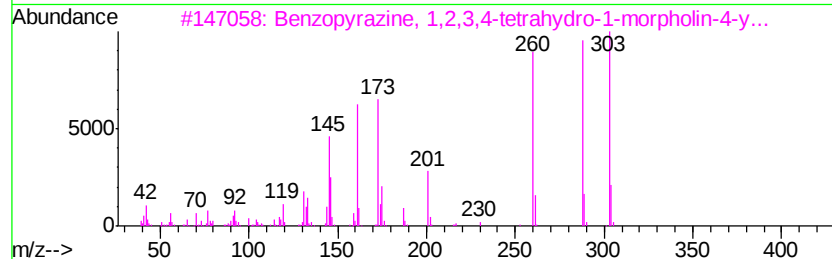
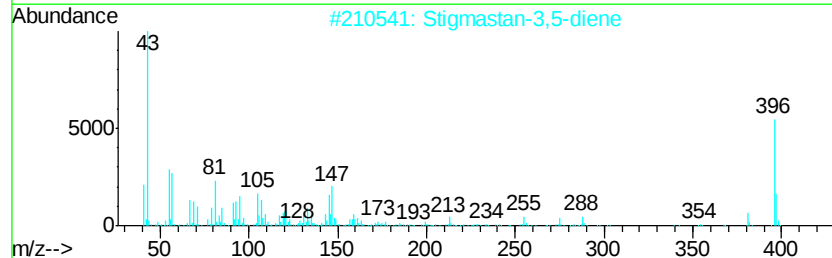
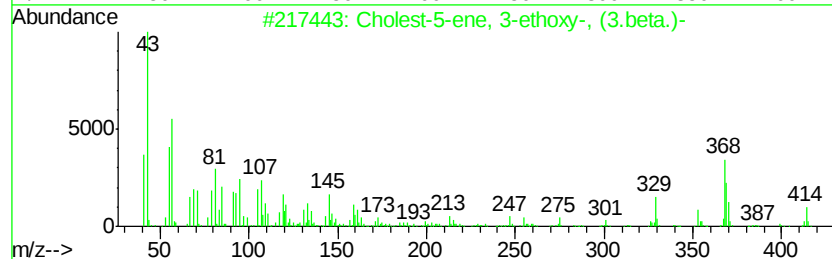
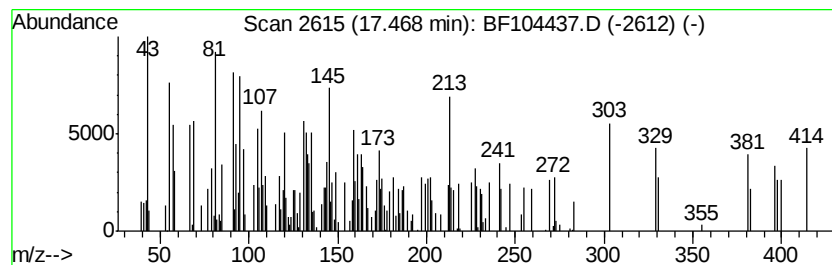
Instrument :
BNA_F
ClientSampleId :
P004-S004-0001-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown17.47 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.		
17.47	5.77 ng	168797	Perylene-d12	15.44		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cholest-5-ene, 3-ethoxy-, (3.bet...	414	C29H50O	000986-19-6	18
2		Stigmastan-3,5-diene	396	C29H48	1000214-16-4	12
3		Benzopyrazine, 1,2,3,4-tetrahydr...	303	C16H21N3O3	342390-29-8	10
4		Imidazo[1,2-a]pyridine-2-methana...	255	C15H14FN3	1000319-53-7	9
5		9.beta.,10.alpha.-Androst-4-en-3...	408	C21H29BrO3	006765-86-2	9



Data Path : Z:\HPCHEM1\BNA F\DATA\BF041118\
Data File : BF104437.D
Acq On : 11 Apr 2018 14:49
Operator : JU/SJ
Sample : J2310-05 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P004-S004-0001-01

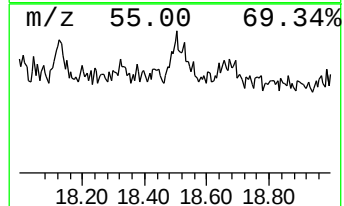
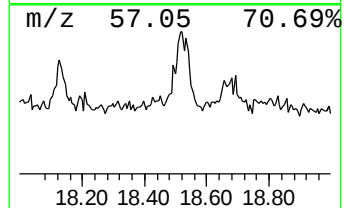
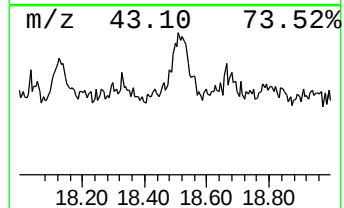
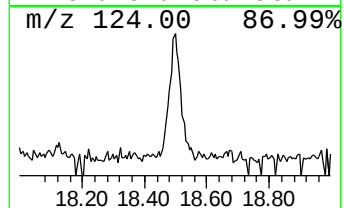
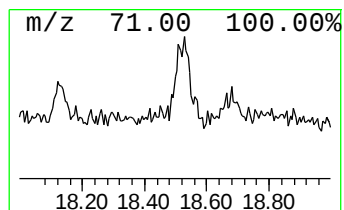
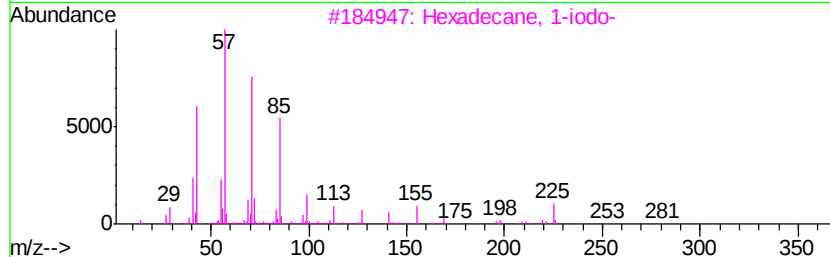
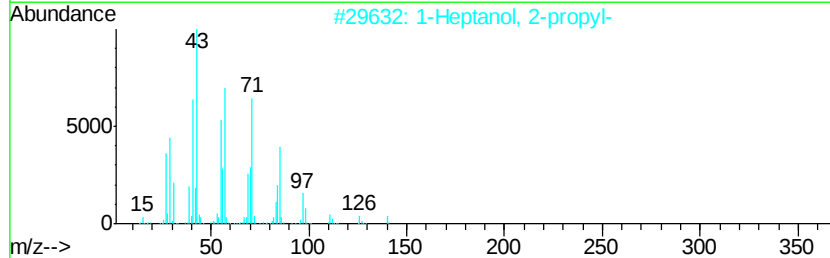
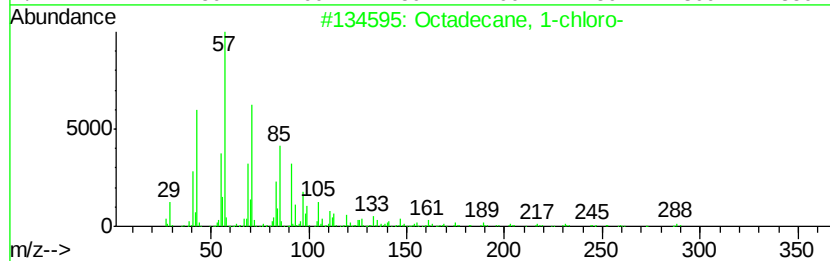
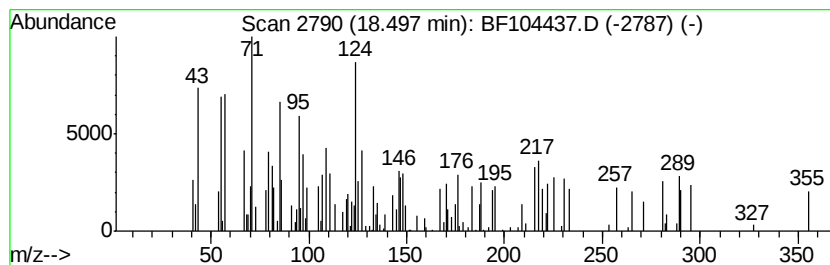
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown18.50 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.50	4.70 ng	137698	Perylene-d12	15.44

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	18
2		1-Heptanol, 2-propyl-	158	C10H22O	010042-59-8	14
3		Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	14
4		Methoxyacetic acid, 2-tetradecyl...	286	C17H34O3	1000282-04-8	14
5		Undecane, 2-methyl-	170	C12H26	007045-71-8	14



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF041118\
Data File : BF104437.D
Acq On : 11 Apr 2018 14:49
Operator : JU/SJ
Sample : J2310-05 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P004-S004-0001-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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
unknown6.57	6.57	36.5	ng	1393010	1	6.80	762490	20.0
n-Hexadecanoic acid	11.86	3.1	ng	120414	4	11.33	771635	20.0
1-Heneicosanol	13.82	4.0	ng	164649	5	13.98	831225	20.0
9-Octadecenamide,...	14.74	5.2	ng	151270	6	15.44	585327	20.0
1-Nonadecene	15.96	3.3	ng	96246	6	15.44	585327	20.0
unknown17.06	17.06	4.8	ng	139343	6	15.44	585327	20.0
unknown17.47	17.47	5.8	ng	168797	6	15.44	585327	20.0
unknown18.50	18.50	4.7	ng	137698	6	15.44	585327	20.0