LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071816\
Data File : BF089098.D
Acq On : 18 Jul 2016 23:11
Operator : UM/SJ
Sample : H4046-27
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C5-5

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-BF063016.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	1.632	3	4	13	rVV	166135	262279	12.67%	1.950%
2	1.747	13	14	38	rVB	1087676	2069349	100.00%	15.386%
3	4.776	277	279	284	rBV	54696	77845	3.76%	0.579%
4	5.244	317	320	322	rBV	768331	1064693	51.45%	7.916%
5	6.296	410	412	415	rBV	807081	1020710	49.33%	7.589%
6	6.410	420	422	425	rVB	988478	1012317	48.92%	7.527%
7	6.639	440	442	444	rBV	350024	292895	14.15%	2.178%
8	6.799	453	456	458	rBB	1049082	902972	43.64%	6.714%
9	7.210	489	492	494	rBV	729866	688759	33.28%	5.121%
10	7.930	552	555	557	rBV	416101	393183	19.00%	2.923%
11	9.005	646	649	651	rBV	1300820	1105639	53.43%	8.221%
12	9.405	681	684	686	rVB	284627	252113	12.18%	1.875%
13	9.679	705	708	710	rBV	319951	345453	16.69%	2.569%
14	10.456	774	776	779	rBV2	455175	497002	24.02%	3.695%
15	10.593	786	788	794	rVB	29001	35755	1.73%	0.266%
16	11.153	834	837	838	rBV	305663	309507	14.96%	2.301%
17	11.393	855	858	863	rBV3	14355	22527	1.09%	0.167%
18	11.702	882	885	886	rBV	49555	55906	2.70%	0.416%
19	12.353	940	942	944	rBV	54964	47193	2.28%	0.351%
20	12.582	959	962	963	rVV2	58927	77366	3.74%	0.575%
21	12.651	963	968	969	rVB3	10386	21405	1.03%	0.159%
22	12.731	973	975	978	rVB	681584	823933	39.82%	6.126%
23	12.799	979	981	985	rBV	12079	26776	1.29%	0.199%
24	12.891	985	989	993	rBV3	15598	41824	2.02%	0.311%
25	12.982	993	997	998	rBV3	17959	40192	1.94%	0.299%
26	13.279	1020	1023	1024	rBV	19360	25910	1.25%	0.193%
27	13.325	1024	1027	1029	rVV3	11775	23218	1.12%	0.173%
28	13.416	1034	1035	1039	rVV2	16502	29572	1.43%	0.220%
29	13.519	1042	1044	1046	rVV3	12556	20871	1.01%	0.155%
30	13.576	1048	1049	1052	rVB2	17944	29251	1.41%	0.217%
31	13.645	1052	1055	1058	rBV2	77403	103728	5.01%	0.771%
32	13.771	1063	1066	1073	rBV2	325641	447063	21.60%	3.324%
33	13.885	1074	1076	1078	rBV3	20597	22100	1.07%	0.164%
34	14.159	1098	1100	1102	rBV	21769	28494	1.38%	0.212%

LSC Area Percent Report

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Instrument : BNA_F
ClientSampleId : C5-5

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-BF063016.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.274	1108	1110	1114	rVB2	67390	96505	4.66%	0.718%
36	14.491	1127	1129	1132	rBV3	16453	24669	1.19%	0.183%
37	14.685	1144	1146	1151	rVB5	25189	33064	1.60%	0.246%
38	14.765	1151	1153	1158	rVV	71392	128490	6.21%	0.955%
39	14.857	1159	1161	1166	rVB2	34184	50831	2.46%	0.378%
40	15.028	1174	1176	1178	rVB	36350	43184	2.09%	0.321%
41	15.074	1178	1180	1182	rBV	41941	50233	2.43%	0.373%
42	15.131	1183	1185	1188	rVV	173449	198433	9.59%	1.475%
43	15.554	1220	1222	1224	rBV	22601	30878	1.49%	0.230%
44	16.525	1304	1307	1311	rBV	206245	373187	18.03%	2.775%
45	16.811	1329	1332	1335	rVB2	36044	78163	3.78%	0.581%
46	17.223	1365	1368	1371	rBV4	30603	65363	3.16%	0.486%
47	18.617	1487	1490	1498	rVB7	15647	58586	2.83%	0.436%

Sum of corrected areas: 13449386

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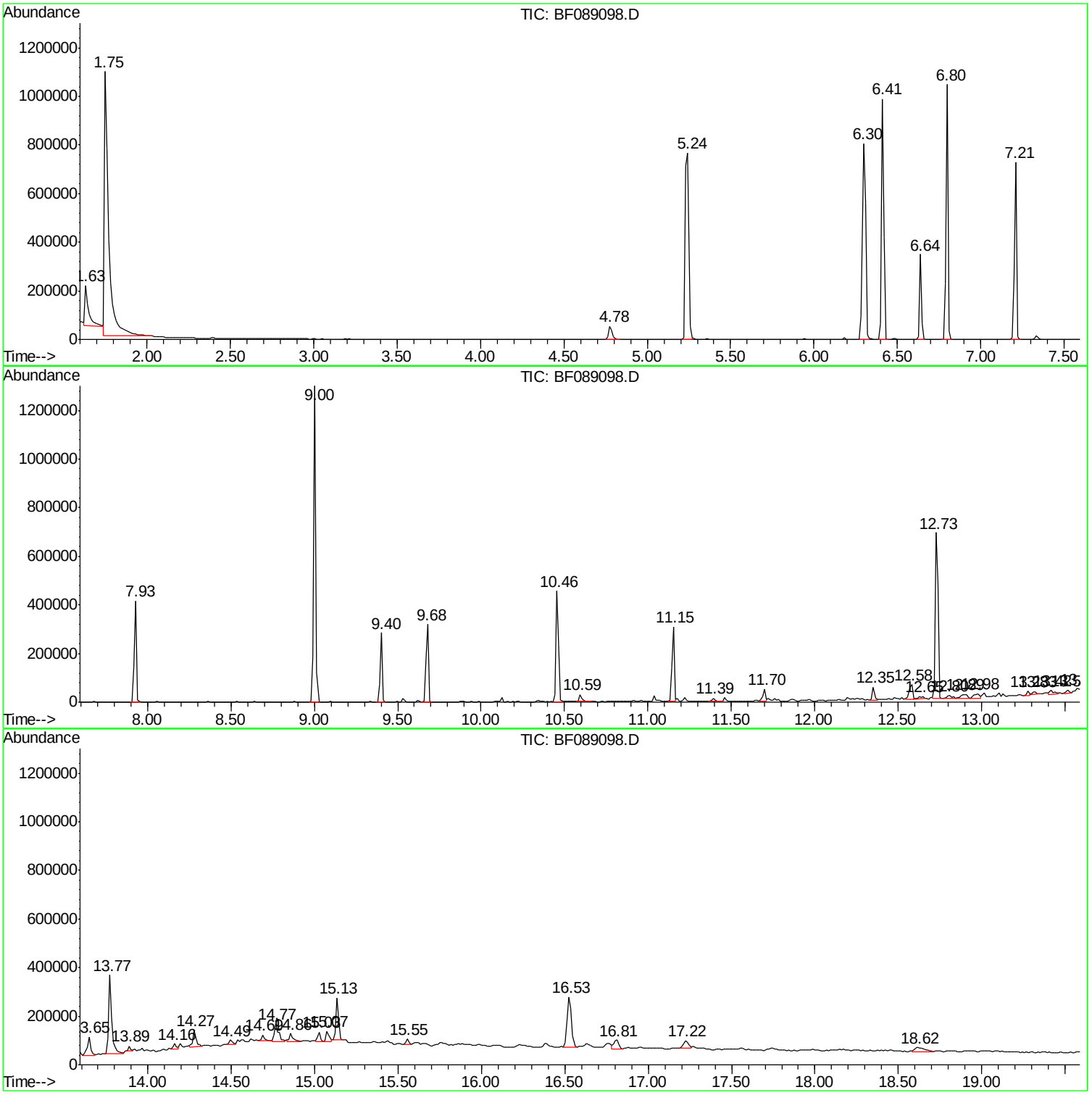
Instrument :
BNA_F
ClientSampleId :
C5-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

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Data File : BF089098.D
Acq On : 18 Jul 2016 23:11
Operator : UM/SJ
Sample : H4046-27
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C5-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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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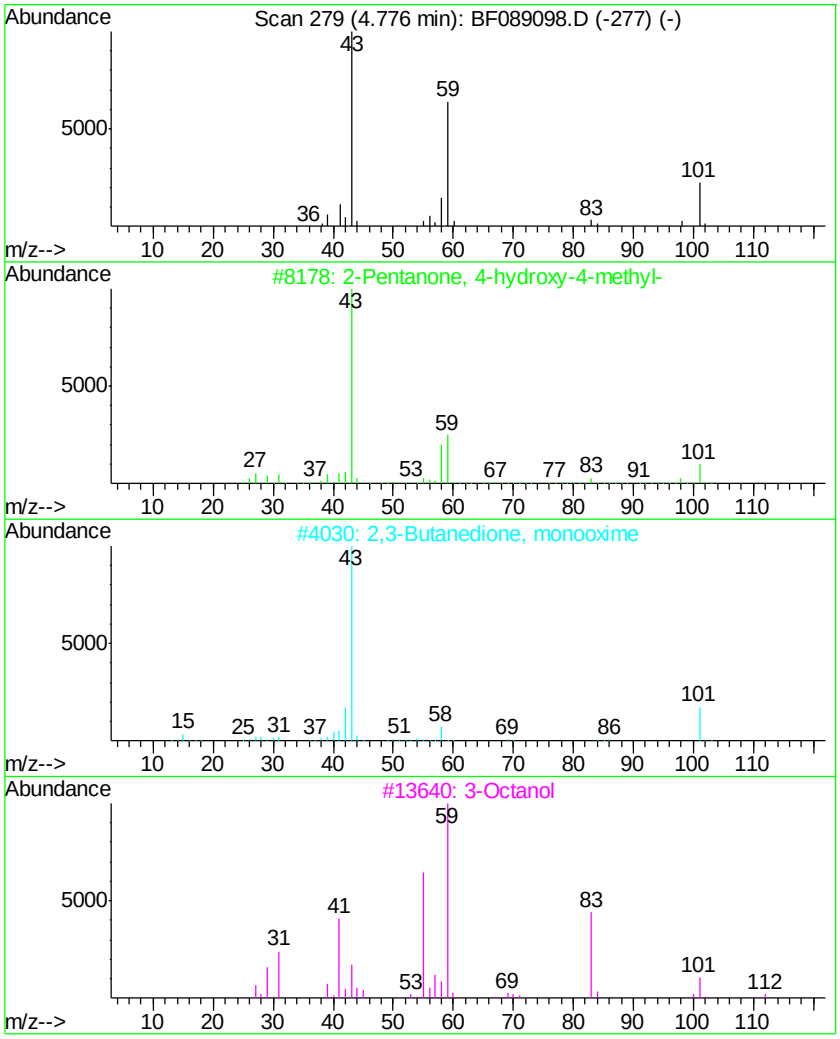
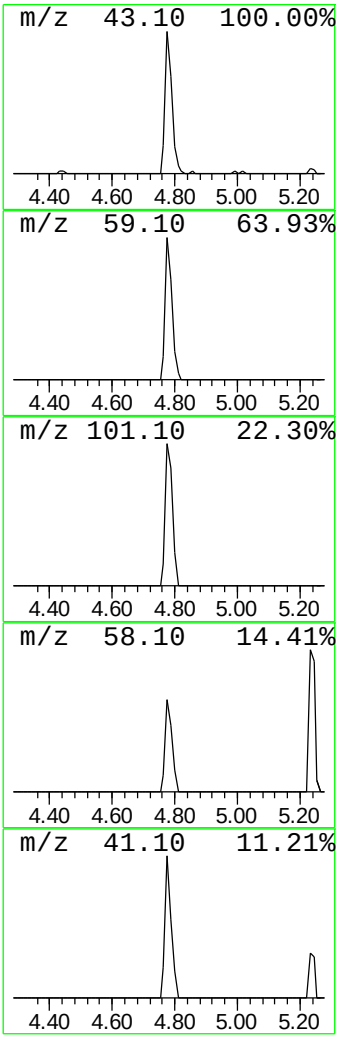
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.78	5.32 ng	77845	1,4-Dichlorobenzene-d4	6.64

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	35
3	3-Octanol	130	C8H18O	000589-98-0	28
4	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	25
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23





Library Search Compound Report

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Data File : BF089098.D
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Operator : UM/SJ
Sample : H4046-27
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C5-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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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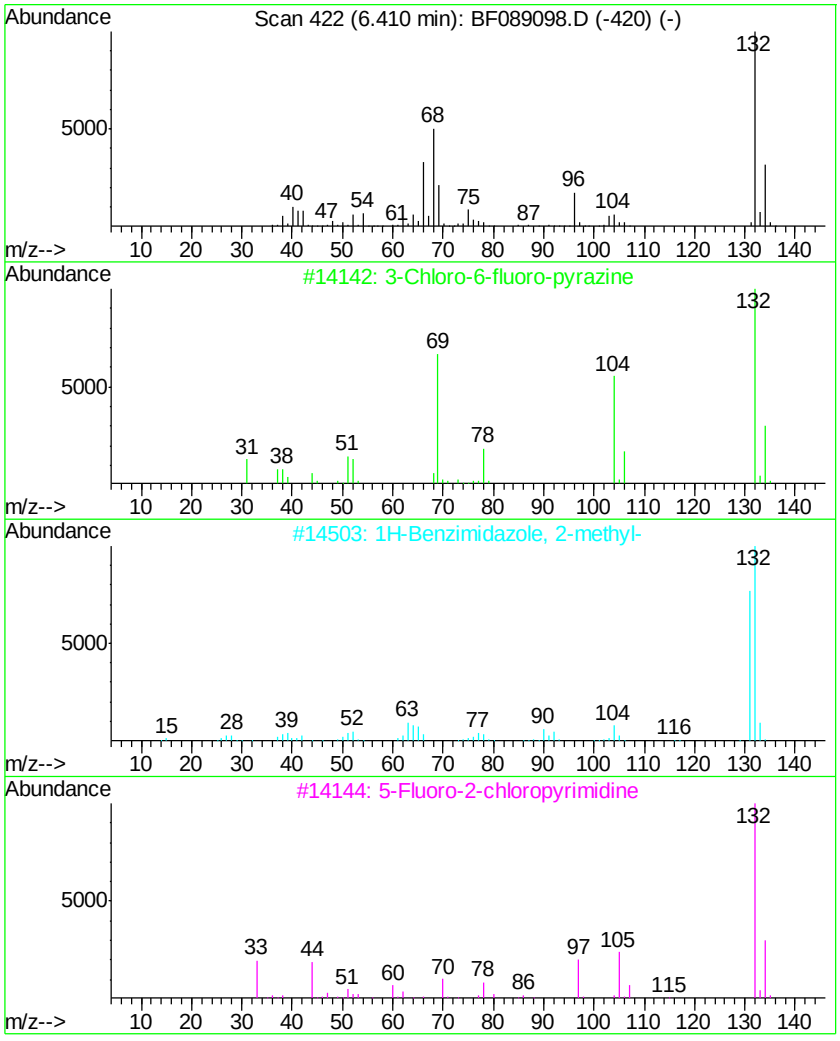
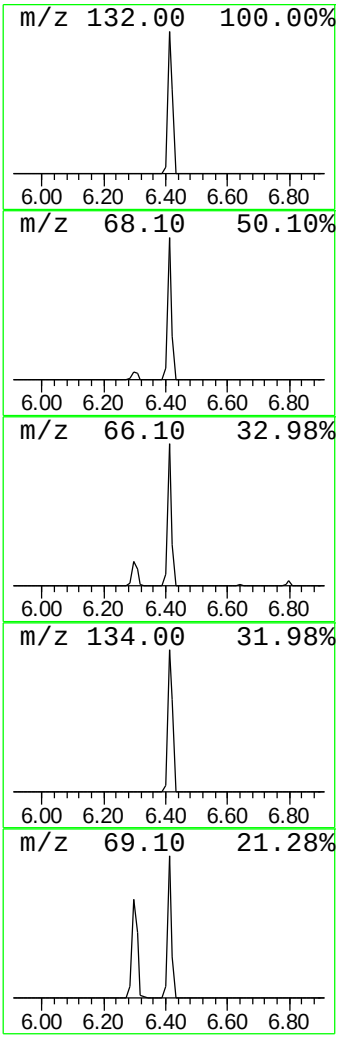
Peak Number 4 unknown6.41 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.41	69.12 ng	1012320	1,4-Dichlorobenzene-d4	6.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
5	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071816\
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Operator : UM/SJ
Sample : H4046-27
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C5-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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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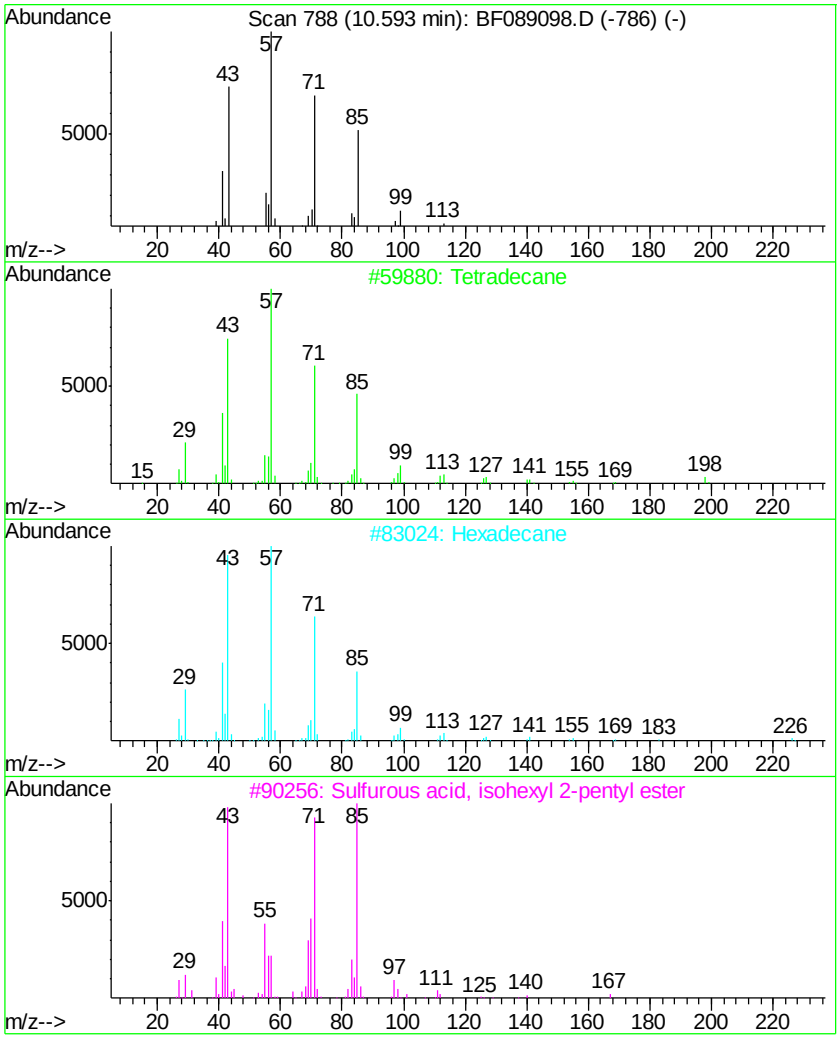
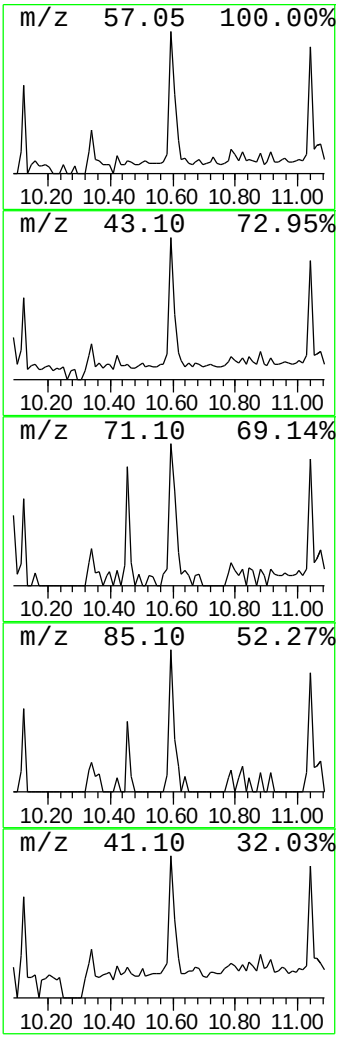
Peak Number 6 Tetradecane Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.59	2.31 ng	35755	Phenanthrene-d10	11.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane	198	C14H30	000629-59-4	80
2	Hexadecane	226	C16H34	000544-76-3	78
3	Sulfurous acid, isohexyl 2-pentyl...	236	C11H24O3S	1000309-15-5	64
4	Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	64
5	3-Ethyl-3-methylheptane	142	C10H22	017302-01-1	64





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Instrument : BNA_F
ClientSampleId : C5-5

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TIC Library : C:\Database\NIST11.L
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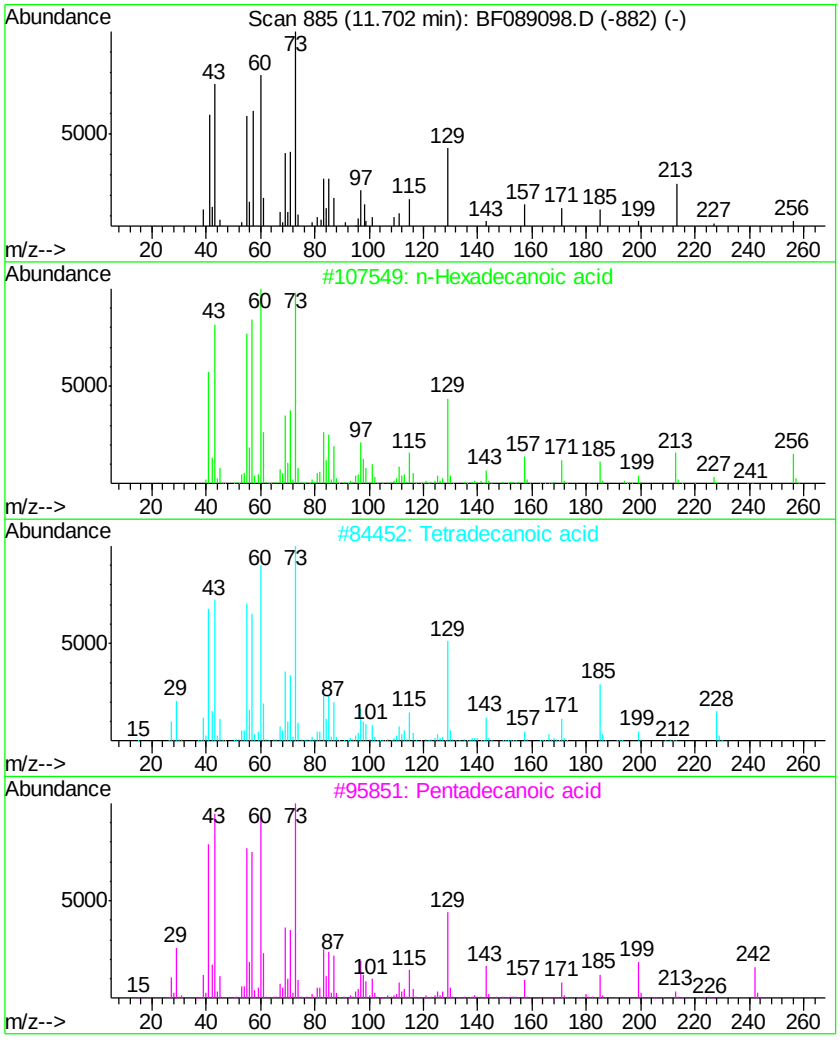
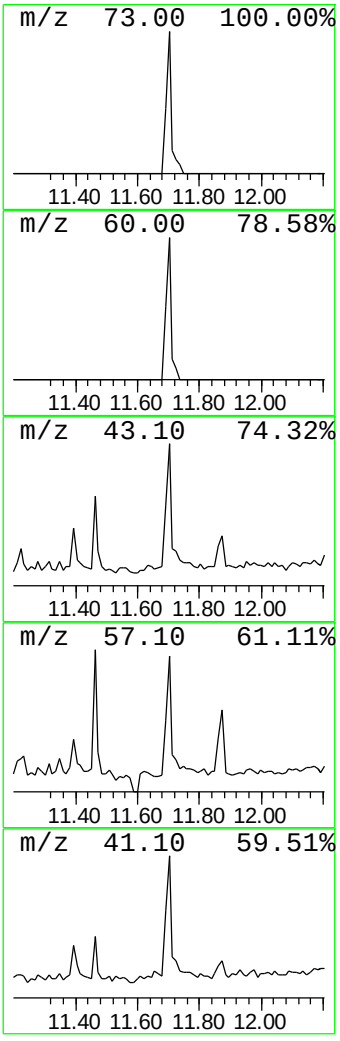
Peak Number 7 n-Hexadecanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.70	3.61 ng	55906	Phenanthrene-d10	11.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	68
4	Tridecanoic acid	214	C13H26O2	000638-53-9	64
5	n-Decanoic acid	172	C10H20O2	000334-48-5	53





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Instrument : BNA_F
ClientSampleId : C5-5

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TIC Library : C:\Database\NIST11.L
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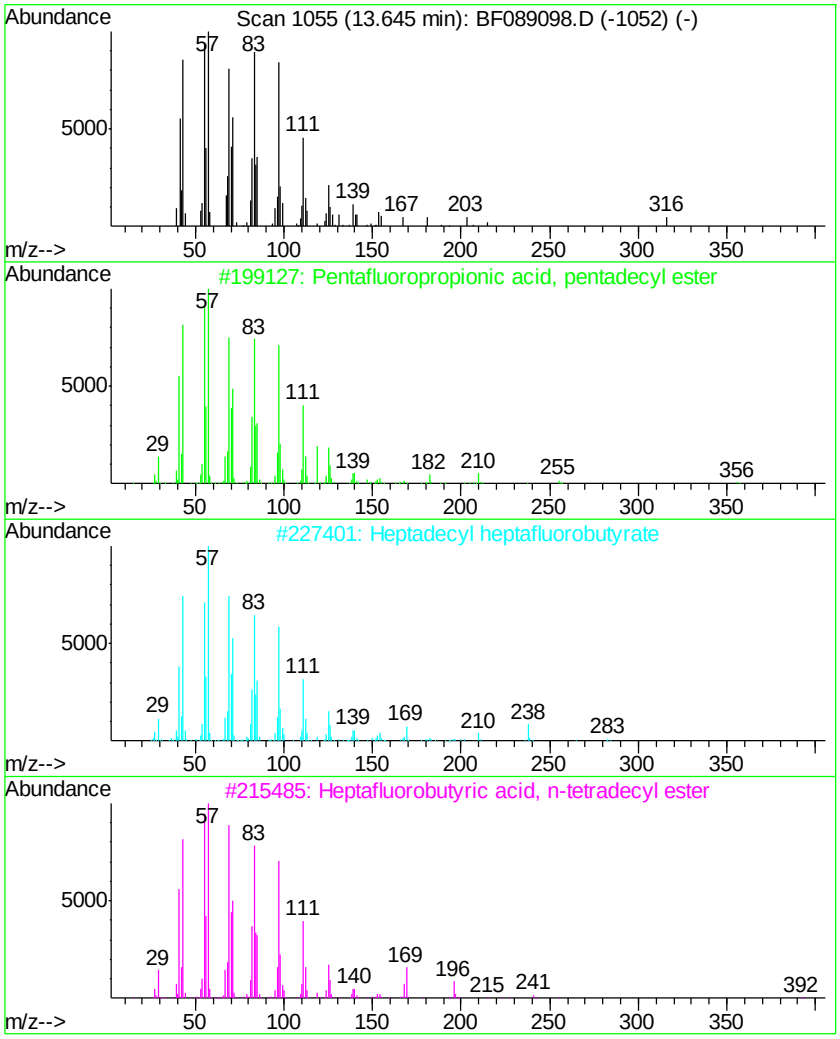
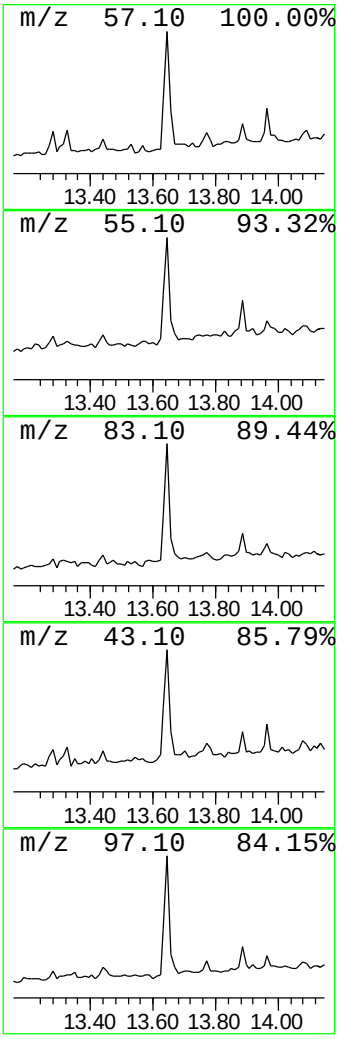
Peak Number 8 Pentafluoropropionic acid, ... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.65	4.64 ng	103728	Chrysene-d12	13.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	95
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	95
3	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	95
4	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	95
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95





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Sample : H4046-27
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Instrument : BNA_F
ClientSampleId : C5-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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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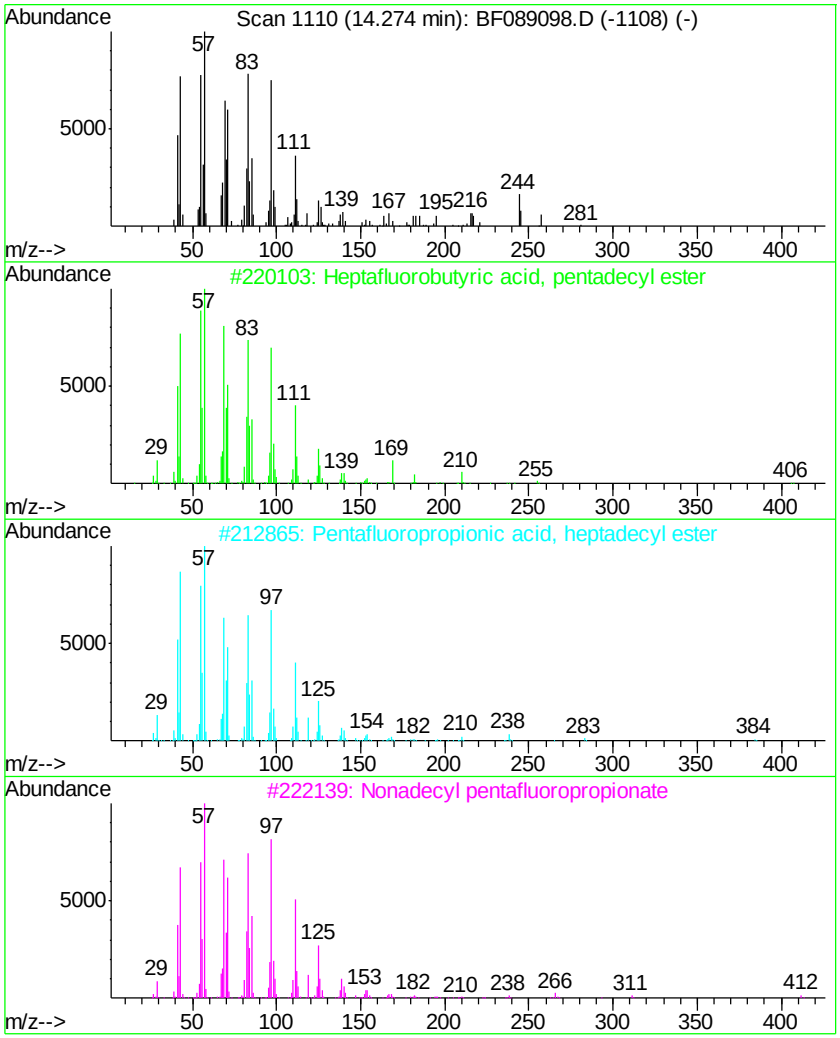
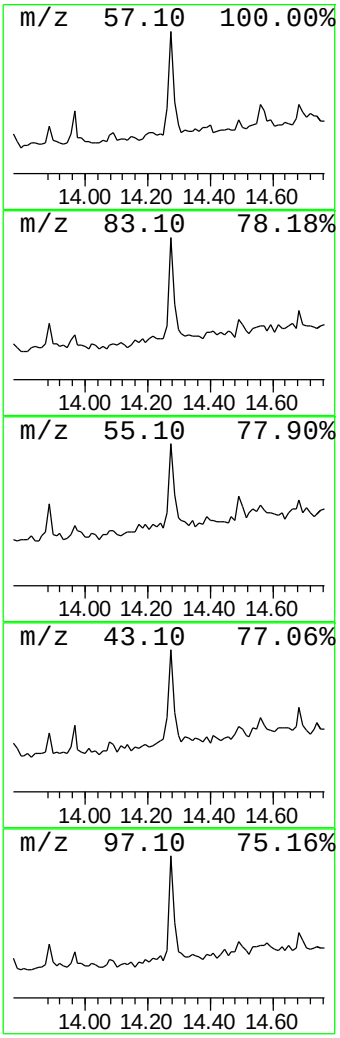
Peak Number 9 Heptafluorobutyric acid, pe... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.27	4.32 ng	96505	Chrysene-d12	13.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93
2	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	90
3	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	90
4	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	90
5	Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	90





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TIC Library : C:\Database\NIST11.L
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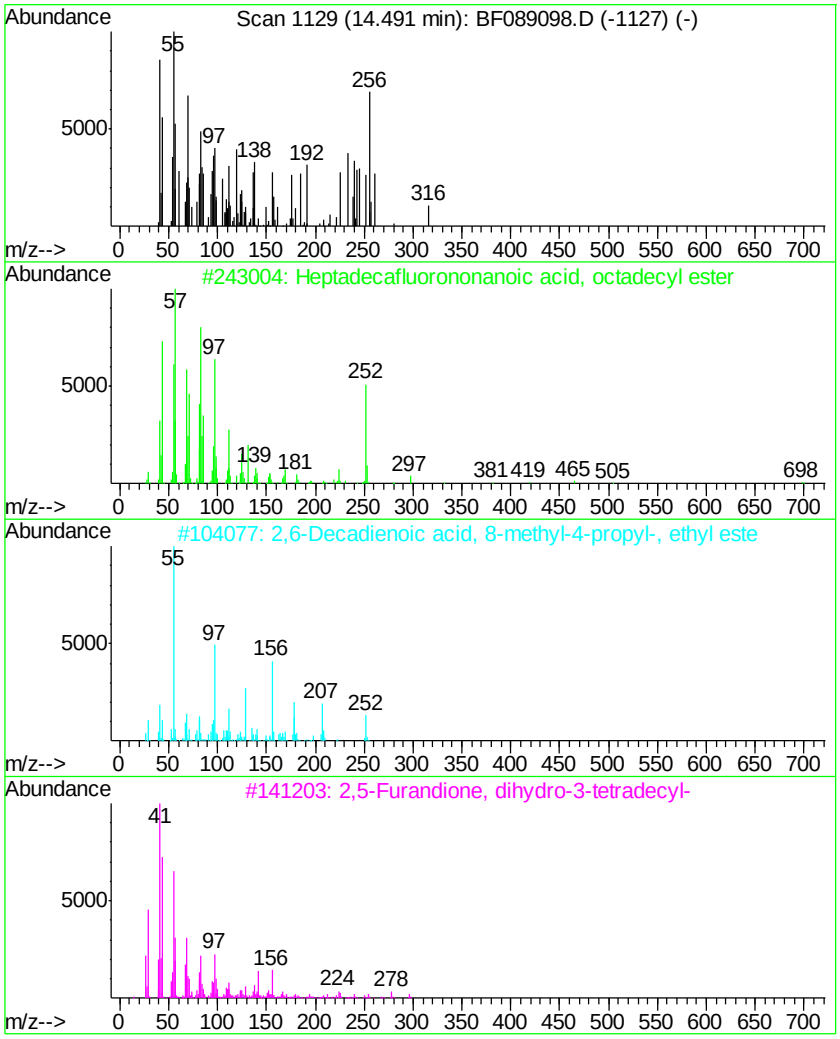
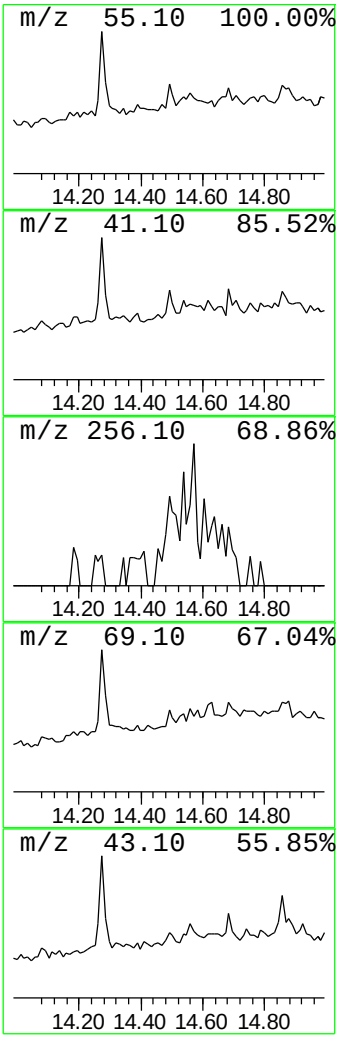
Peak Number 10 unknown14.49 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.49	2.49 ng	24669	Perylene-d12	15.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecafluorononanoic acid, oc...	716	C27H37F17O2	1000356-03-4	10
2	2,6-Decadienoic acid, 8-methyl-4...	252	C16H28O2	056771-51-8	10
3	2,5-Furandione, dihydro-3-tetrad...	296	C18H32O3	047165-57-1	10
4	1-Isoquinolinamine, 3,4-dihydro-...	271	C15H17N3S	1000319-43-3	10
5	8,9,10,11-Tetrahydrobenzo[k]fluo...	256	C20H16	033942-81-3	10





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Instrument : BNA_F
ClientSampleId : C5-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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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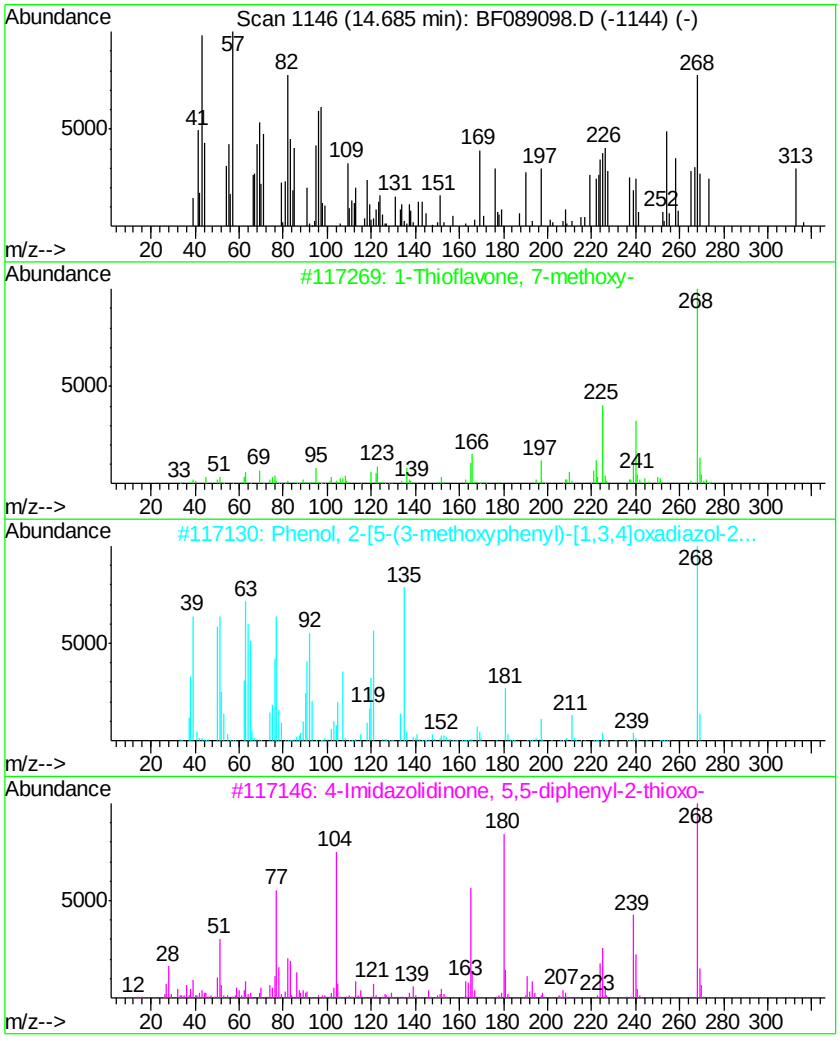
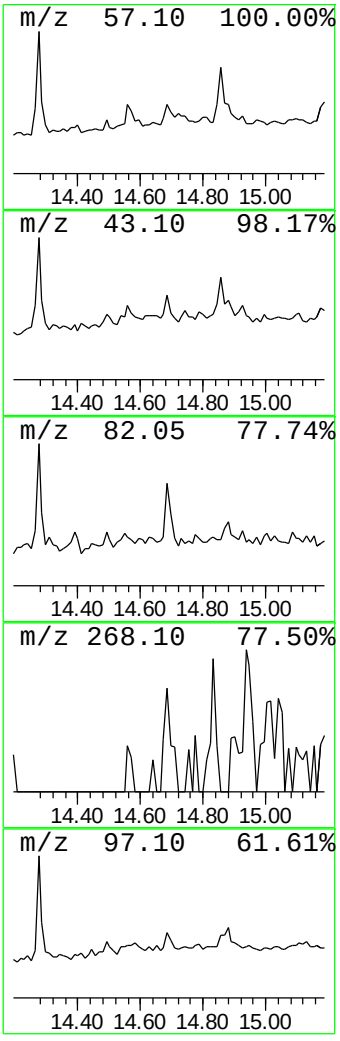
Peak Number 11 unknown14.69 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.69	3.33 ng	33064	Perylene-d12	15.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Thioflavone, 7-methoxy-	268	C16H12O2S	000789-78-6	14
2	Phenol, 2-[5-(3-methoxyphenyl)-[...	268	C15H12N2O3	1000303-05-4	11
3	4-Imidazolidinone, 5,5-diphenyl-...	268	C15H12N2OS	021083-47-6	11
4	2,5-Cyclohexadiene-1,4-dione, 3-...	180	C10H12O3	004586-58-7	10
5	4H-1-Benzopyran-4-one, 3-hydroxy...	268	C16H12O4	007478-60-6	10





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Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C5-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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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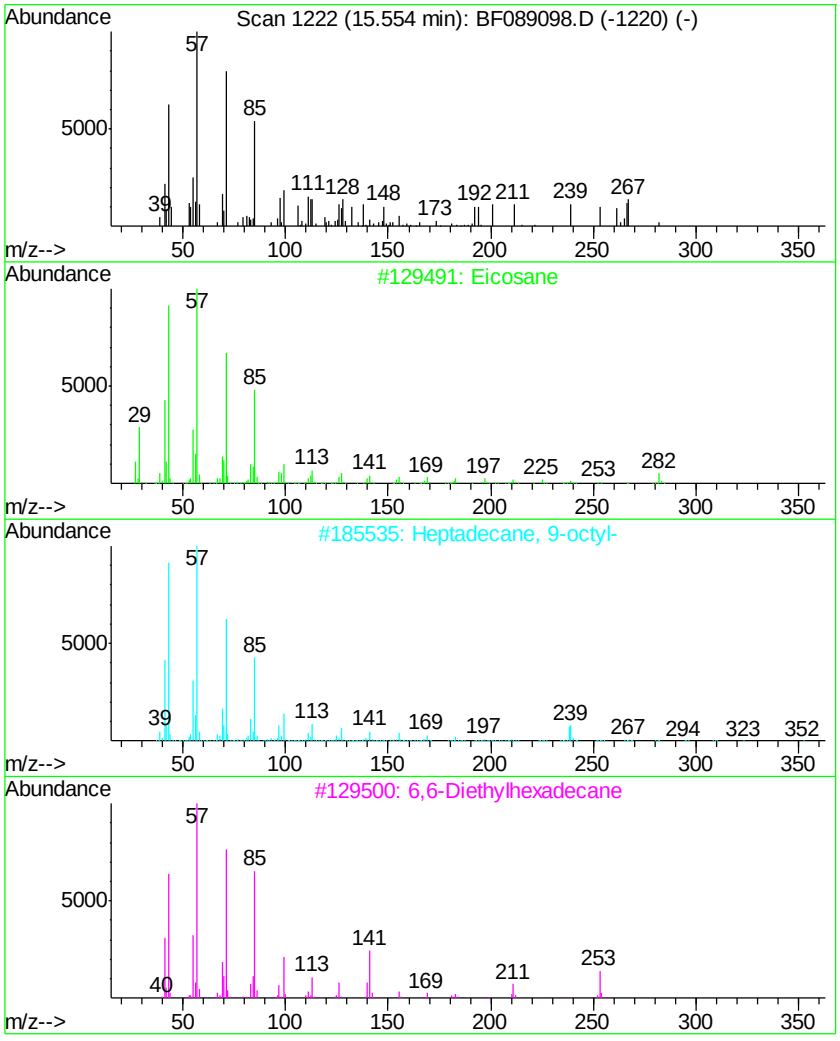
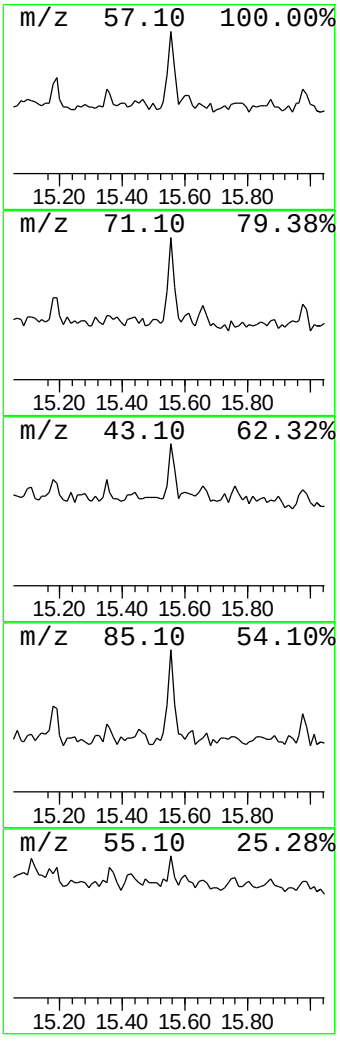
Peak Number 13 Eicosane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.55	3.11 ng	30878	Perylene-d12	15.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	60
2	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	50
3	6,6-Diethylhexadecane	282	C20H42	1000360-41-4	50
4	Hexatriacontane	507	C36H74	000630-06-8	47
5	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	47





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071816\
Data File : BF089098.D
Acq On : 18 Jul 2016 23:11
Operator : UM/SJ
Sample : H4046-27
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C5-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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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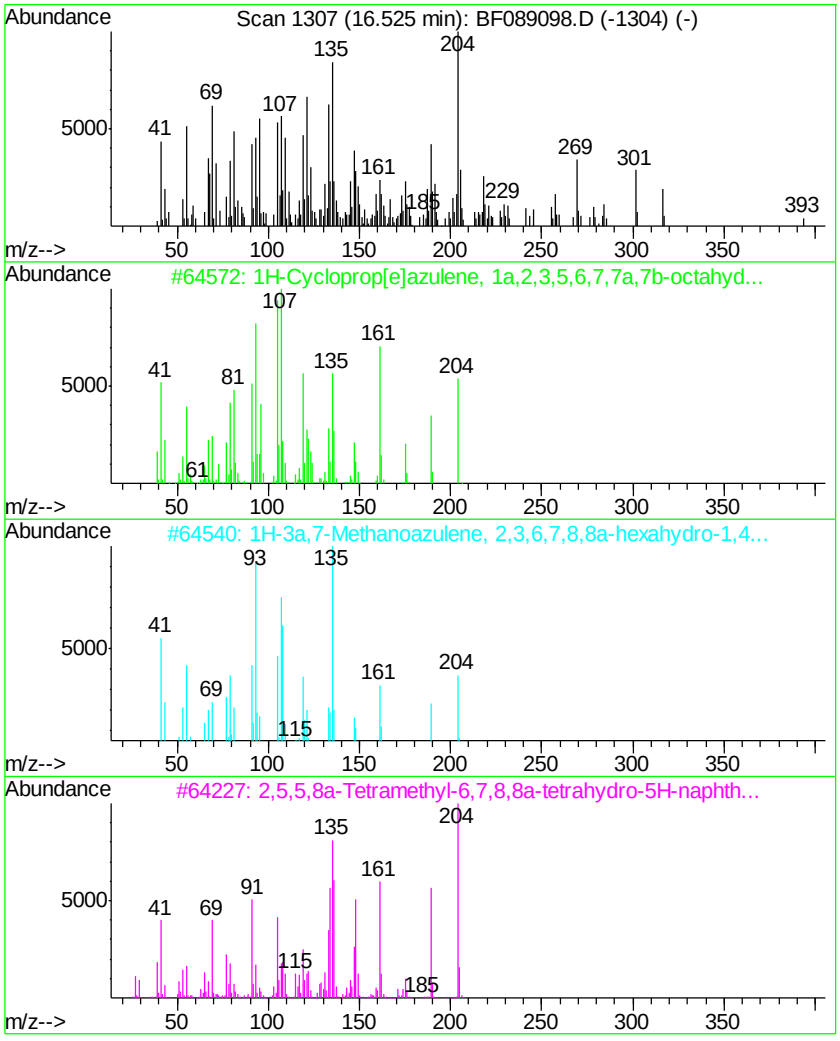
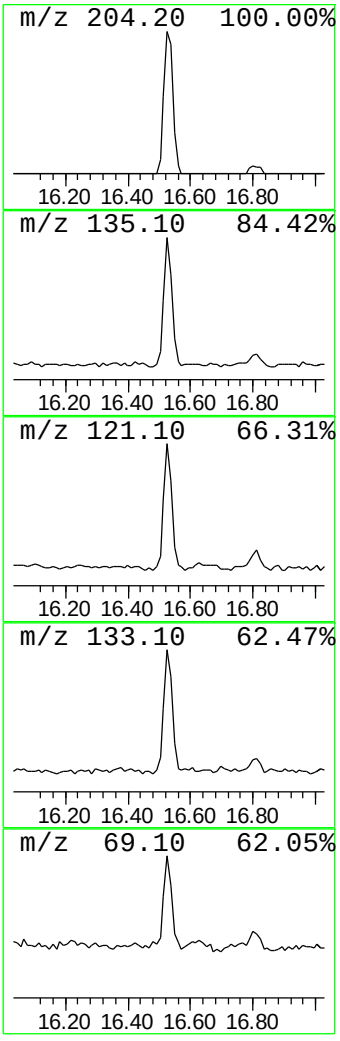
Peak Number 14 1H-Cycloprop[e]azulene, 1a,... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.53	37.61 ng	373187	Perylene-d12	15.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Cycloprop[e]azulene, 1a,2,3,5...	204	C15H24	021747-46-6	55
2	1H-3a,7-Methanoazulene, 2,3,6,7,...	204	C15H24	000560-32-7	52
3	2,5,5,8a-Tetramethyl-6,7,8,8a-te...	204	C14H20O	124957-09-1	49
4	Farnesyl bromide	284	C15H25Br	006874-67-5	49
5	Guaia-3,9-diene	204	C15H24	000489-83-8	46





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Data File : BF089098.D
Acq On : 18 Jul 2016 23:11
Operator : UM/SJ
Sample : H4046-27
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C5-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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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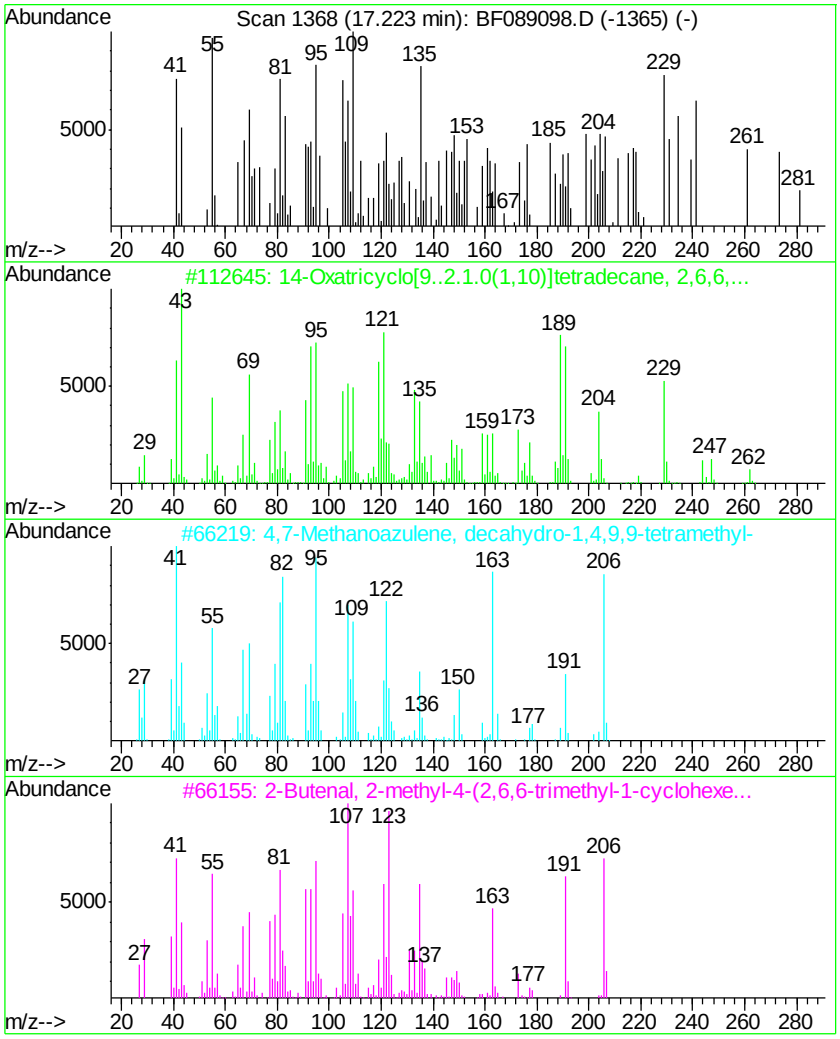
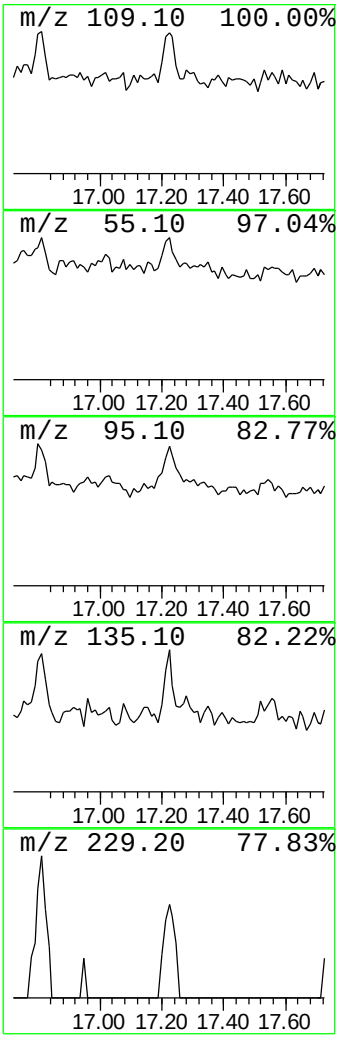
Peak Number 15 unknown17.22 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.22	6.59 ng	65363	Perylene-d12	15.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	14-Oxatricyclo[9..2.1.0(1,10)]te...	262	C18H30O	1000193-06-8	25
2	4,7-Methanoazulene, decahydro-1,...	206	C15H26	020478-88-0	14
3	2-Butenal, 2-methyl-4-(2,6,6-tri...	206	C14H22O	003155-71-3	11
4	4-(3,4-Methylenedioxyphenyl)-2-b...	192	C11H12O3	055418-52-5	11
5	Anthracene, tetradecahydro-, (4a...	192	C14H24	019128-78-0	11





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071816\
Data File : BF089098.D
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Operator : UM/SJ
Sample : H4046-27
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C5-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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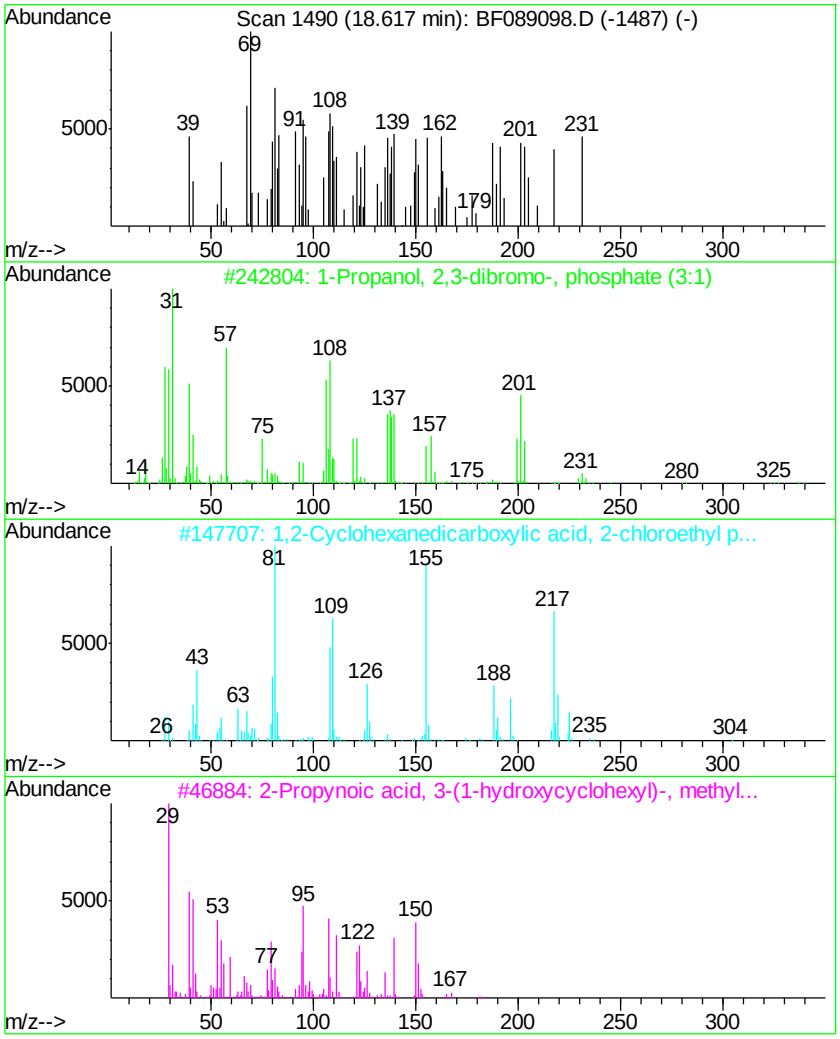
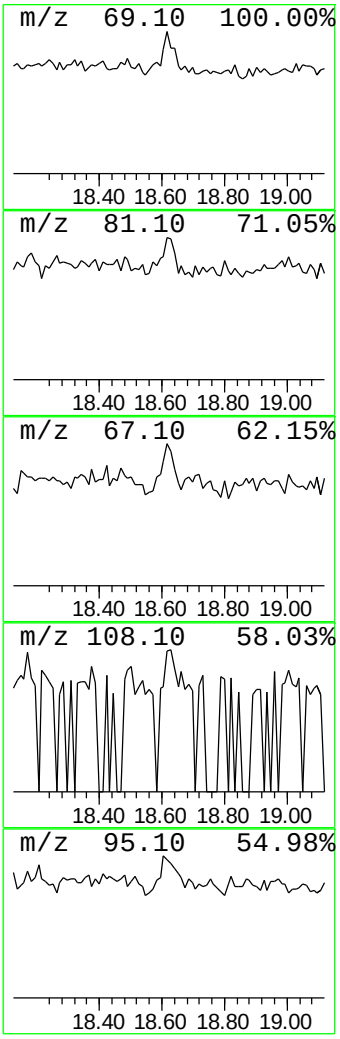
Peak Number 16 unknown18.62 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.62	5.90 ng	58586	Perylene-d12	15.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol, 2,3-dibromo-, phosph...	692	C9H15Br6O4P	000126-72-7	10
2	1,2-Cyclohexanedicarboxylic acid...	304	C15H25ClO4	1000340-04-3	9
3	2-Propynoic acid, 3-(1-hydroxycy...	182	C10H14O3	1000317-29-4	9
4	O,O-Diethyl S-eththionylmethyl p...	260	C7H17O4PS2	002588-05-8	2
5	Bisethoxo(methoxo)oxovanadium	188	C5H13O4V	062450-00-4	2





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071816\
Data File : BF089098.D
Acq On : 18 Jul 2016 23:11
Operator : UM/SJ
Sample : H4046-27
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C5-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.78	5.3	ng	77845	1	6.64	292895	20.0
unknown6.41	6.41	69.1	ng	1012320	1	6.64	292895	20.0
Tetradecane	10.59	2.3	ng	35755	4	11.15	309507	20.0
n-Hexadecanoic acid	11.70	3.6	ng	55906	4	11.15	309507	20.0
Pentafluoropropio...	13.65	4.6	ng	103728	5	13.77	447063	20.0
Heptafluorobutyri...	14.27	4.3	ng	96505	5	13.77	447063	20.0
unknown14.49	14.49	2.5	ng	24669	6	15.13	198433	20.0
unknown14.69	14.69	3.3	ng	33064	6	15.13	198433	20.0
Eicosane	15.55	3.1	ng	30878	6	15.13	198433	20.0
1H-Cycloprop[e]az...	16.53	37.6	ng	373187	6	15.13	198433	20.0
unknown17.22	17.22	6.6	ng	65363	6	15.13	198433	20.0
unknown18.62	18.62	5.9	ng	58586	6	15.13	198433	20.0