LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072717\
Data File : BF097139.D
Acq On : 27 Jul 2017 23:01
Operator : SJ/JU
Sample : I4424-10 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AU-06-072417-D

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-BF072517.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	4.616	461	464	476	rBV	132850	187122	11.76%	1.500%
2	5.081	540	543	557	rBV	1472569	1591768	100.00%	12.756%
3	6.145	720	724	739	rBV	1399846	1376221	86.46%	11.028%
4	6.257	739	743	753	rVB	1496503	1300984	81.73%	10.425%
5	6.486	778	782	794	rBV	440685	367475	23.09%	2.945%
6	6.639	804	808	816	rBV	1136028	992856	62.37%	7.956%
7	7.051	874	878	892	rBV	1005257	874254	54.92%	7.006%
8	7.192	899	902	910	rVB	17122	22417	1.41%	0.180%
9	7.769	996	1000	1005	rBV	632066	519713	32.65%	4.165%
10	8.845	1179	1183	1186	rBV	1514529	1205640	75.74%	9.661%
11	9.245	1247	1251	1256	rBV	238963	189447	11.90%	1.518%
12	9.510	1293	1296	1301	rBV	429212	415590	26.11%	3.330%
13	9.945	1364	1370	1372	rBV2	46042	48380	3.04%	0.388%
14	9.969	1372	1374	1380	rVB	22208	17625	1.11%	0.141%
15	10.298	1426	1430	1437	rVB	645721	559308	35.14%	4.482%
16	10.439	1451	1454	1461	rBV2	42735	49870	3.13%	0.400%
17	10.886	1526	1530	1532	rBV	27364	22995	1.44%	0.184%
18	10.986	1543	1547	1550	rBV	397143	334029	20.98%	2.677%
19	11.010	1550	1551	1555	rVV	50433	29204	1.83%	0.234%
20	11.069	1557	1561	1565	rVB2	16304	19431	1.22%	0.156%
21	11.310	1599	1602	1608	rVB	17228	17760	1.12%	0.142%
22	12.051	1720	1728	1729	rBV4	9337	16887	1.06%	0.135%
23	12.192	1749	1752	1755	rBV	108951	87870	5.52%	0.704%
24	12.416	1785	1790	1795	rBV	94380	90966	5.71%	0.729%
25	12.568	1812	1816	1820	rVB	847045	722373	45.38%	5.789%
26	12.815	1852	1858	1862	rBV4	13437	17797	1.12%	0.143%
27	13.480	1967	1971	1978	rVB3	30437	43965	2.76%	0.352%
28	13.610	1988	1993	1996	rBV	407752	430421	27.04%	3.449%
29	13.633	1996	1997	2002	rVB2	60079	43500	2.73%	0.349%
30	13.715	2007	2011	2014	rBV6	14062	22646	1.42%	0.181%
31	14.027	2061	2064	2067	rBV4	14106	19734	1.24%	0.158%
32	14.409	2126	2129	2136	rBV7	23212	49119	3.09%	0.394%
33	14.468	2136	2139	2144	rVV7	18004	24201	1.52%	0.194%
34	14.604	2158	2162	2168	rVB	61330	96030	6.03%	0.770%

LSC Area Percent Report

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Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AU-06-072417-D

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-BF072517.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.692	2174	2177	2180	rBV2	25486	28644	1.80%	0.230%
36	14.851	2202	2204	2210	rVB	35978	41080	2.58%	0.329%
37	14.904	2211	2213	2218	rVB	45118	49383	3.10%	0.396%
38	14.957	2218	2222	2225	rBV	275565	286148	17.98%	2.293%
39	15.192	2261	2262	2266	rBV4	18489	17399	1.09%	0.139%
40	15.362	2288	2291	2295	rVB3	28591	37185	2.34%	0.298%
41	15.398	2295	2297	2305	rBV9	25877	47849	3.01%	0.383%
42	15.633	2335	2337	2340	rBV4	18739	24094	1.51%	0.193%
43	15.733	2351	2354	2356	rBV3	21920	30168	1.90%	0.242%
44	16.903	2549	2553	2554	rBV4	12986	17651	1.11%	0.141%
45	18.156	2764	2766	2772	rBV7	15261	18035	1.13%	0.145%
46	18.262	2783	2784	2791	rBV7	17723	30518	1.92%	0.245%
47	18.721	2856	2862	2863	rBV4	22190	43141	2.71%	0.346%

Sum of corrected areas: 12478893

LSC Report - Integrated Chromatogram

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Data File : BF097139.D
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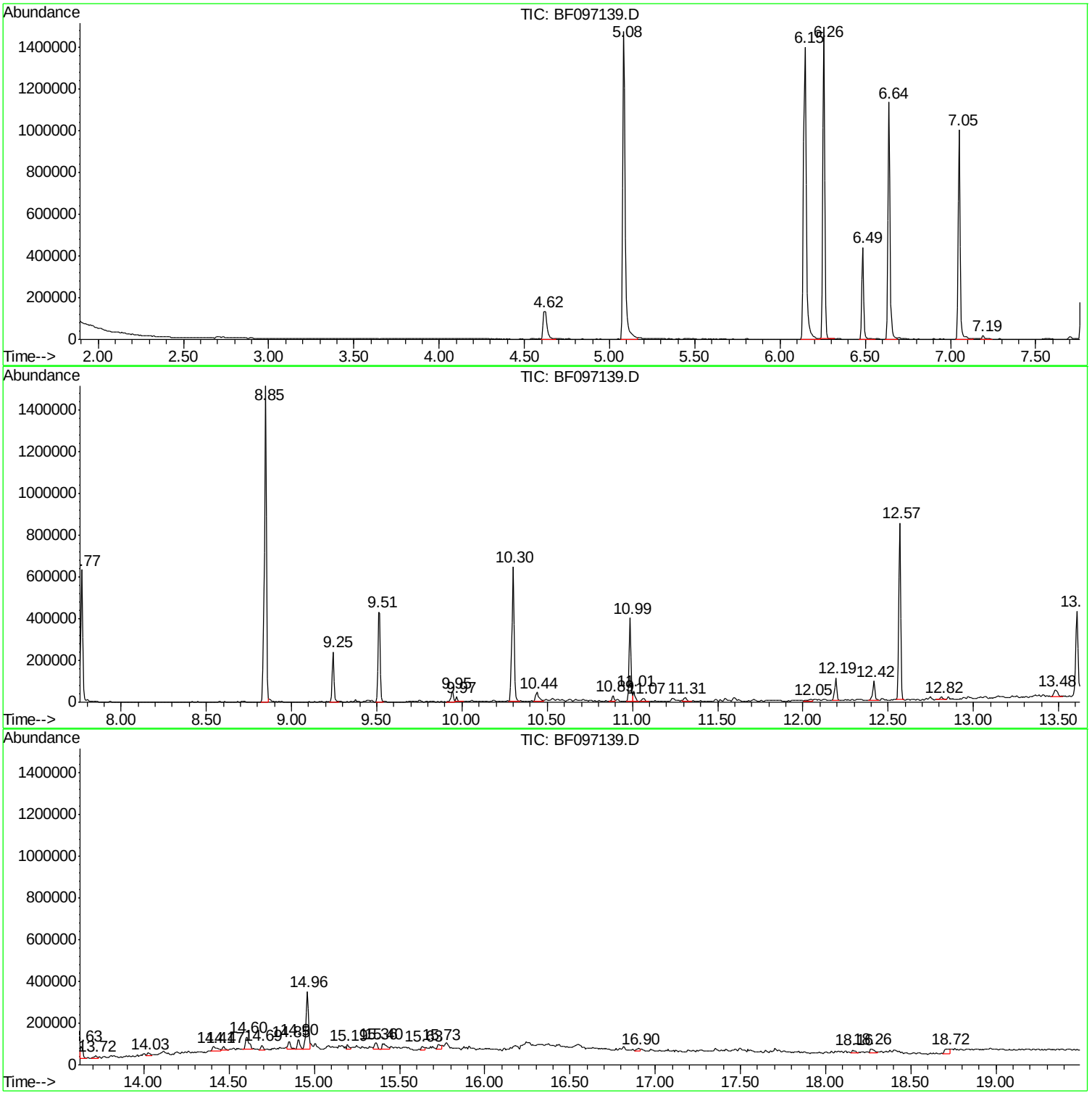
Operator : SJ/JU
Sample : I4424-10 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AU-06-072417-D

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.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

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072717\
Data File : BF097139.D
Acq On : 27 Jul 2017 23:01
Operator : SJ/JU
Sample : I4424-10 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AU-06-072417-D

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

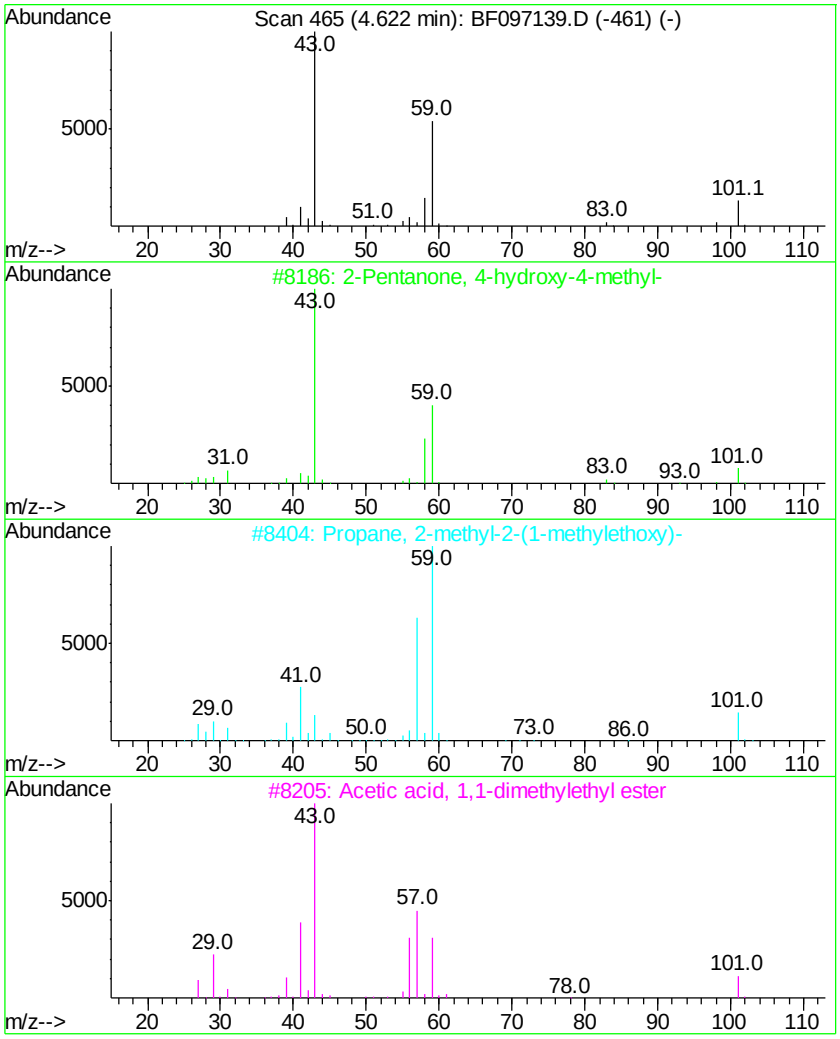
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

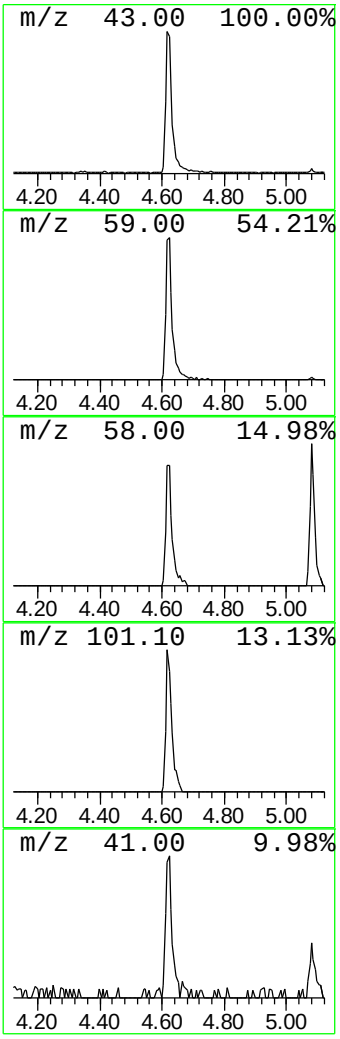
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.62	10.18 ng	187122	1,4-Dichlorobenzene-d4	6.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
4	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9
5	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF072717\
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Acq On : 27 Jul 2017 23:01
Operator : SJ/JU
Sample : I4424-10 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AU-06-072417-D

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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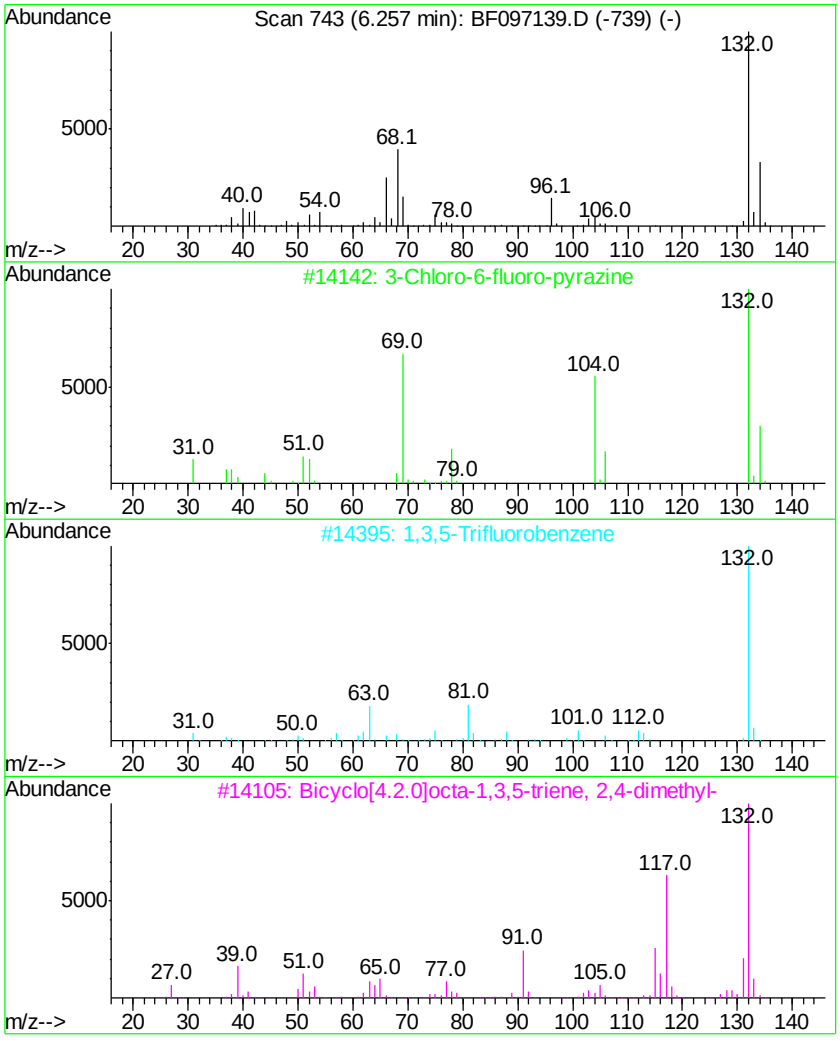
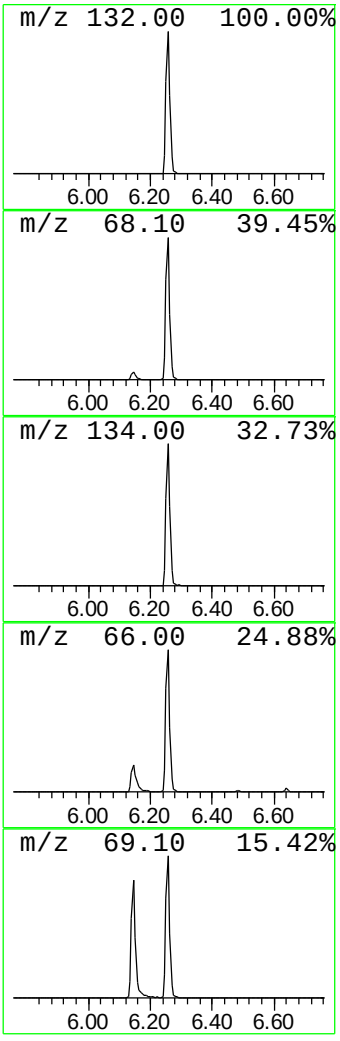
Peak Number 2 unknown6.26 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.26	70.81 ng	1300980	1,4-Dichlorobenzene-d4	6.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF072717\
Data File : BF097139.D
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Operator : SJ/JU
Sample : I4424-10 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AU-06-072417-D

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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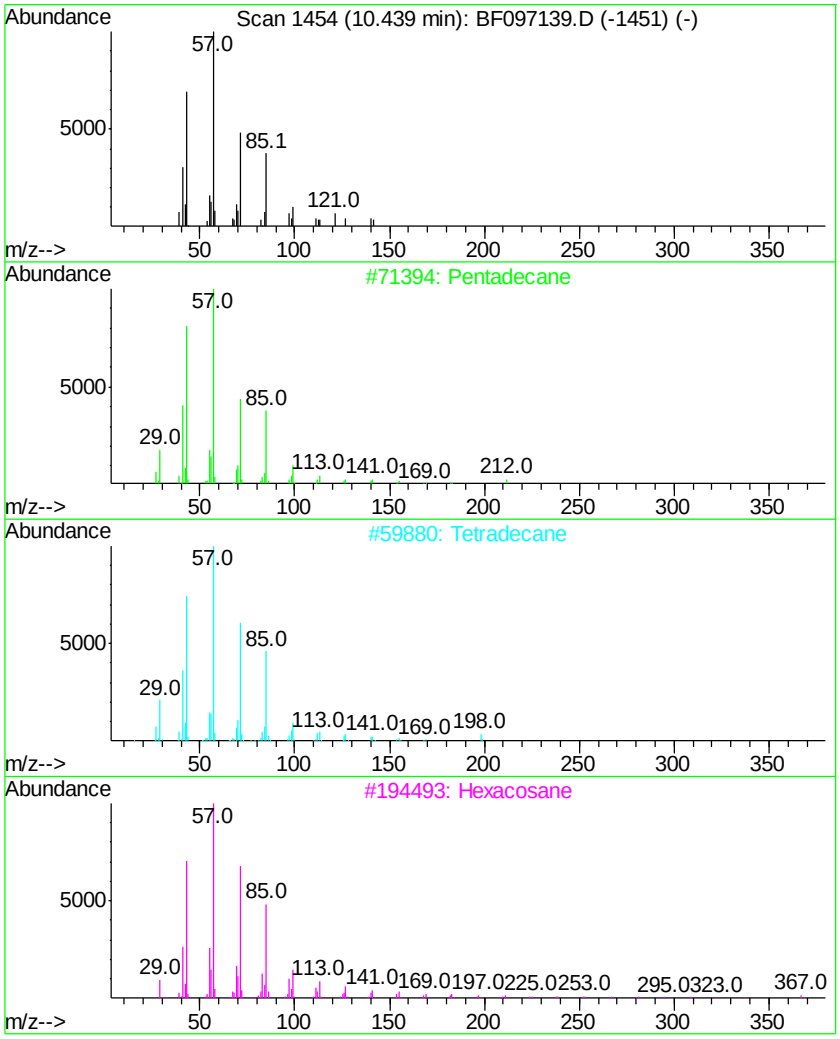
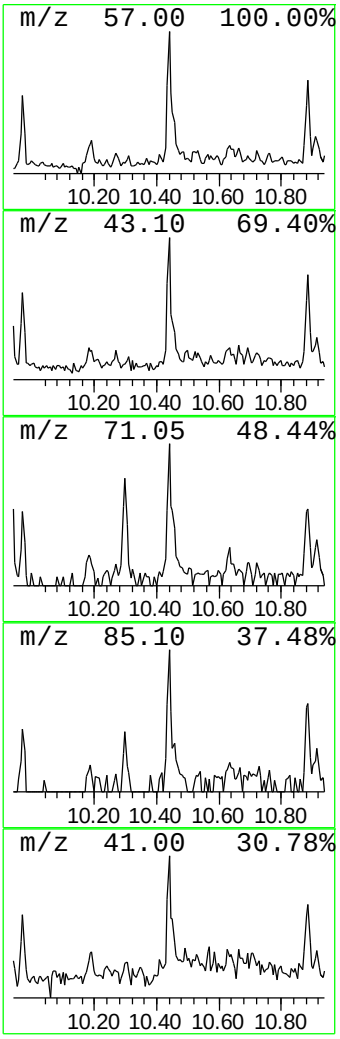
Peak Number 4 Pentadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.44	2.99 ng	49870	Phenanthrene-d10	10.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane	212	C15H32	000629-62-9	86
2	Tetradecane	198	C14H30	000629-59-4	86
3	Hexacosane	366	C26H54	000630-01-3	83
4	Hexatriacontane	507	C36H74	000630-06-8	80
5	Heneicosane	296	C21H44	000629-94-7	72





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Sample : I4424-10 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AU-06-072417-D

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.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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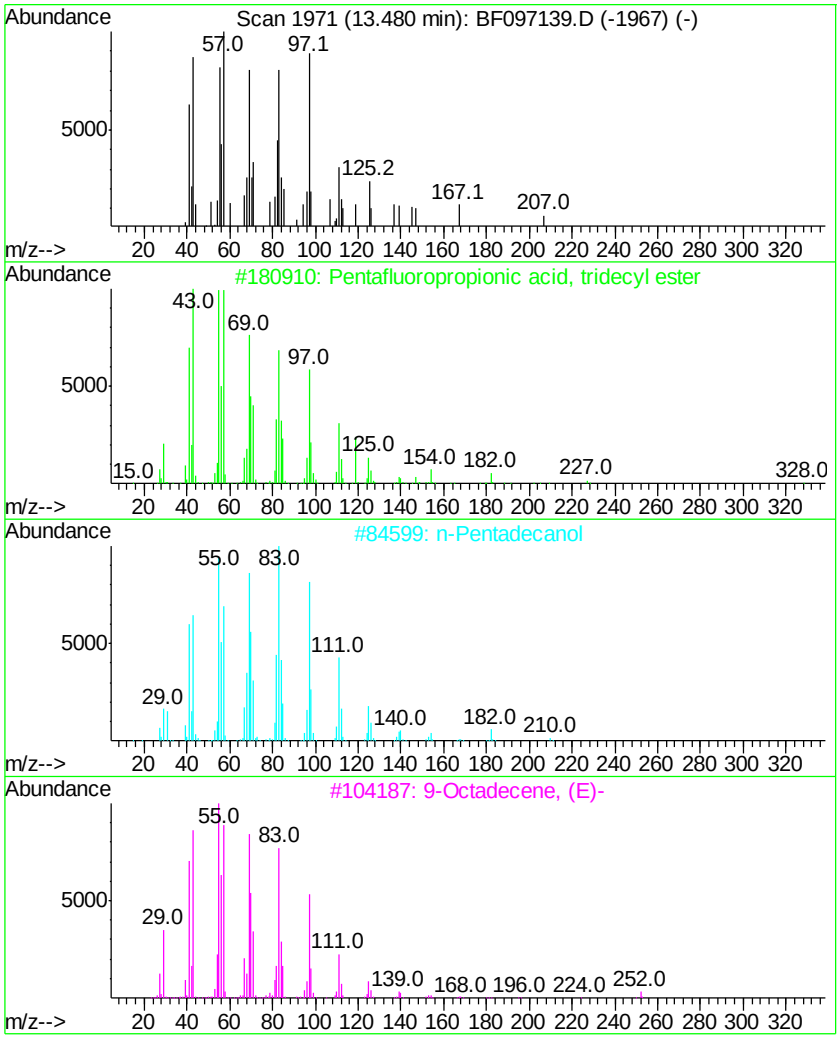
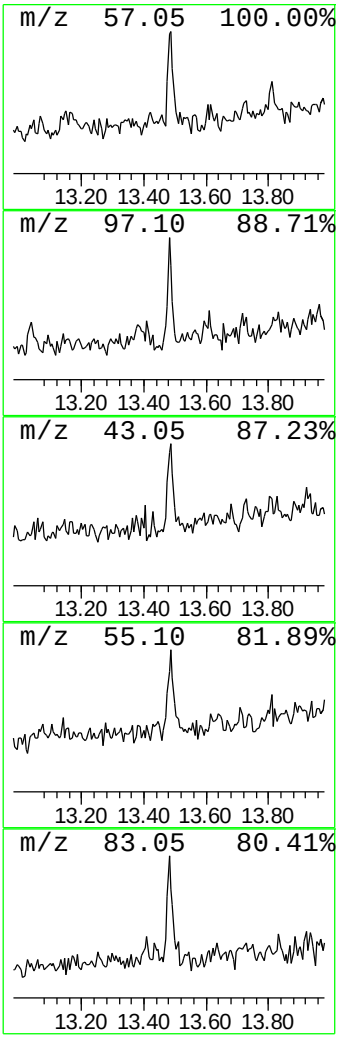
Peak Number 5 Pentafluoropropionic acid, ... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.48	2.04 ng	43965	Chrysene-d12	13.61

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, tride...	346	C16H27F5O2	959261-22-4	72
2	n-Pentadecanol	228	C15H32O	000629-76-5	72
3	9-Octadecene, (E)-	252	C18H36	007206-25-9	64
4	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	58
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	58





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Misc :
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Instrument : BNA_F
ClientSampleId : AU-06-072417-D

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
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TIC Library : C:\DATABASE\NIST11.L
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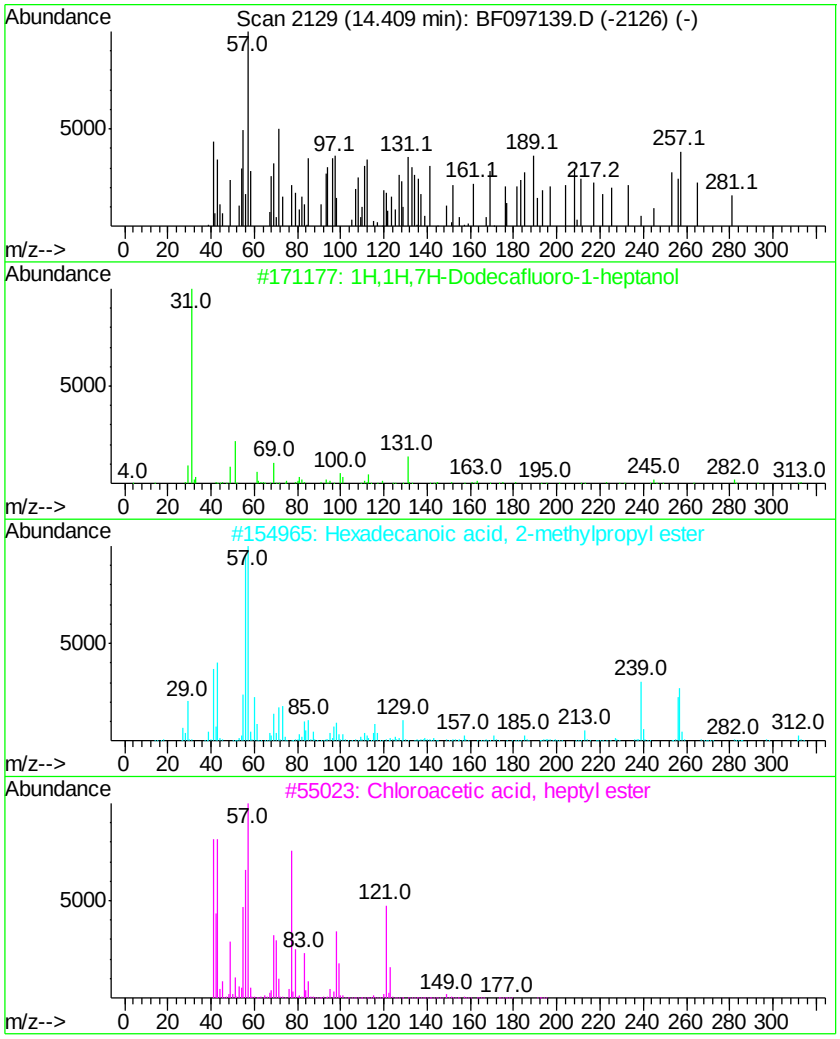
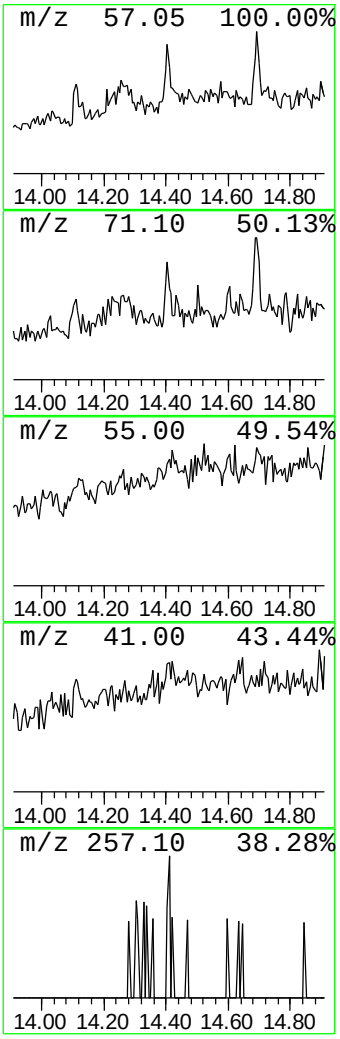
Peak Number 6 unknown14.41 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.41	3.43 ng	49119	Perylene-d12	14.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H,1H,7H-Dodecafluoro-1-heptanol	332	C7H4F12O	000335-99-9	9
2	Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	9
3	Chloroacetic acid, heptyl ester	192	C9H17ClO2	034589-22-5	8
4	Chloroacetic acid, 3-chloropropy...	170	C5H8Cl2O2	062116-55-6	4
5	Acetamide, 2-chloro-N-(2-cyanoet...	146	C5H7ClN2O	017756-81-9	4





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

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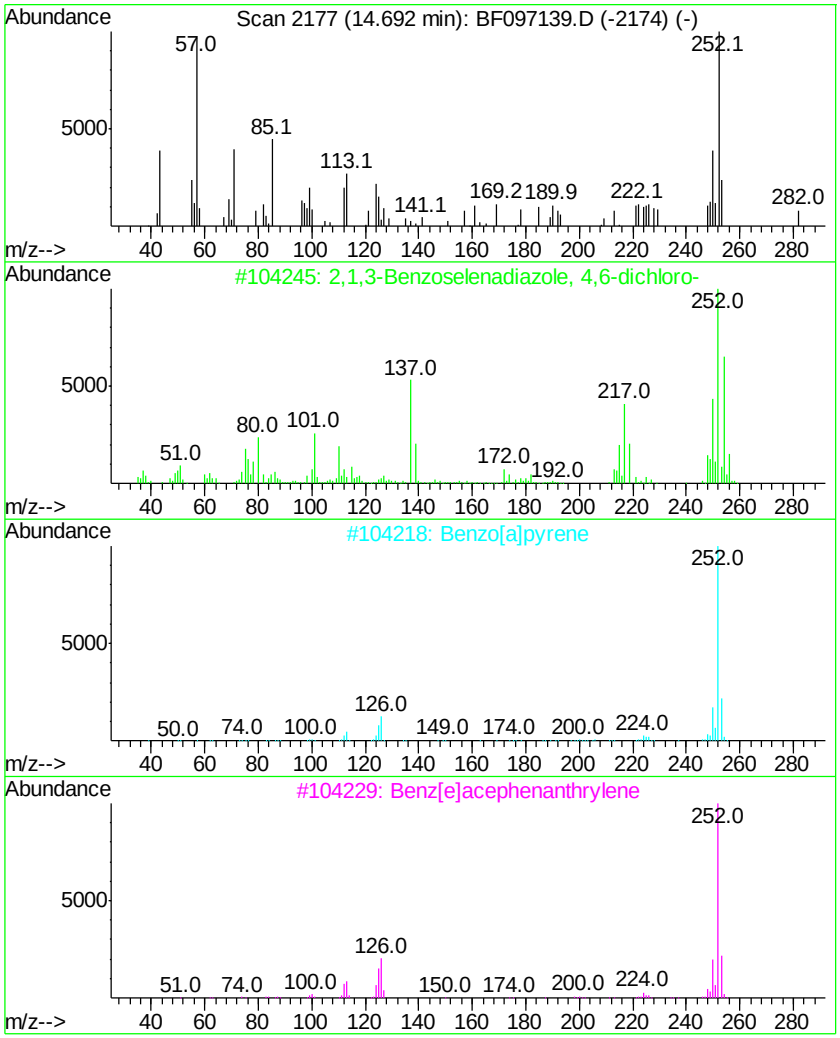
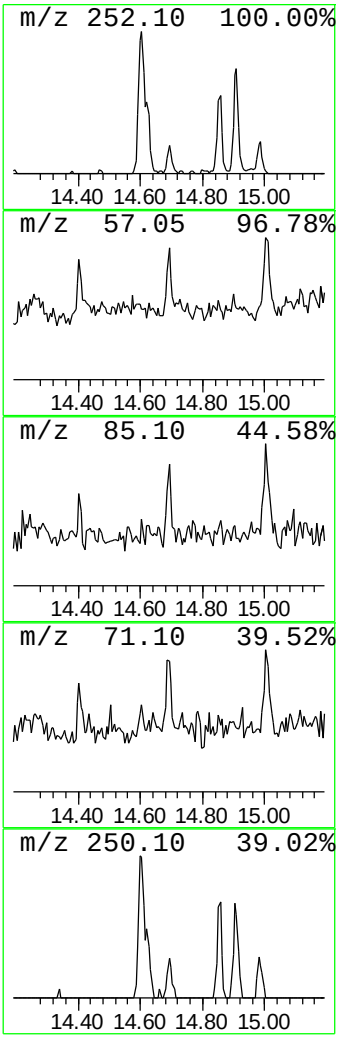
Peak Number 7 unknown14.69 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.69	2.00 ng	28644	Perylene-d12	14.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,1,3-Benzoselenadiazole, 4,6-di...	252	C6H2Cl2N2Se	090030-99-2	49
2	Benzo[a]pyrene	252	C20H12	000050-32-8	43
3	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	38
4	(1-Cyclopentenyl)ferrocene	252	C15H16Fe	012260-67-2	38
5	Benzo[b]naphtho[2,3-d]thiophene,...	252	C17H16S	024964-06-5	38





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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.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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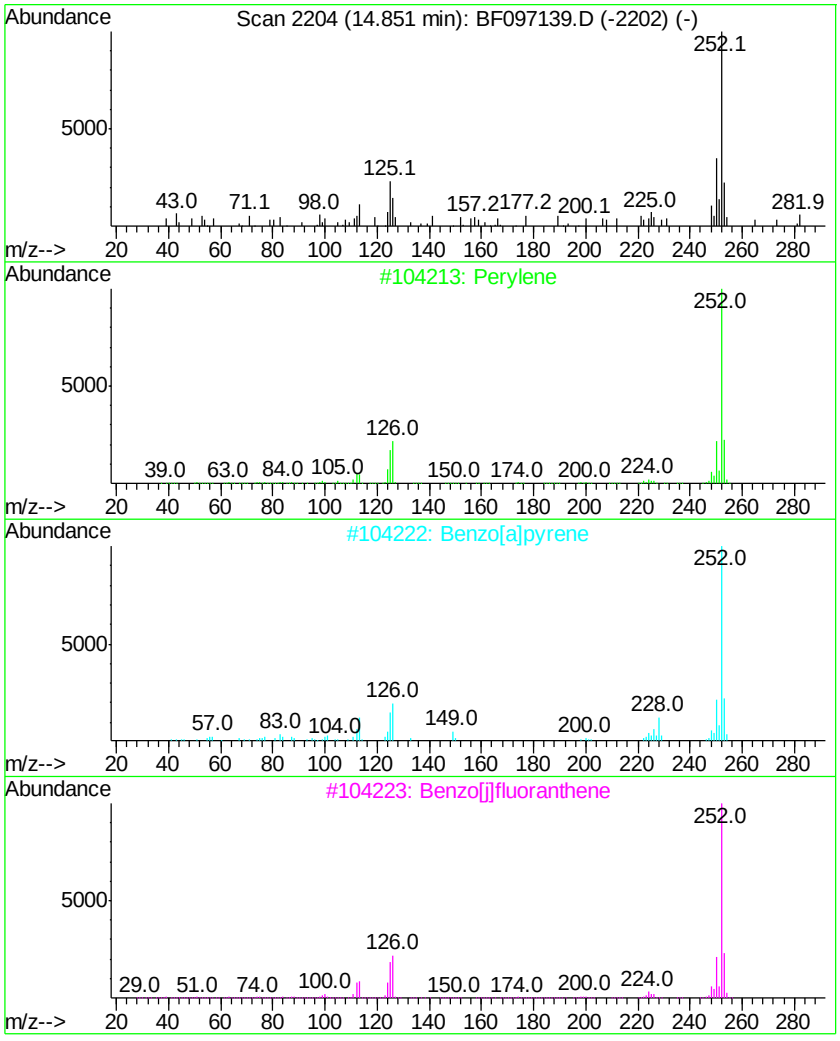
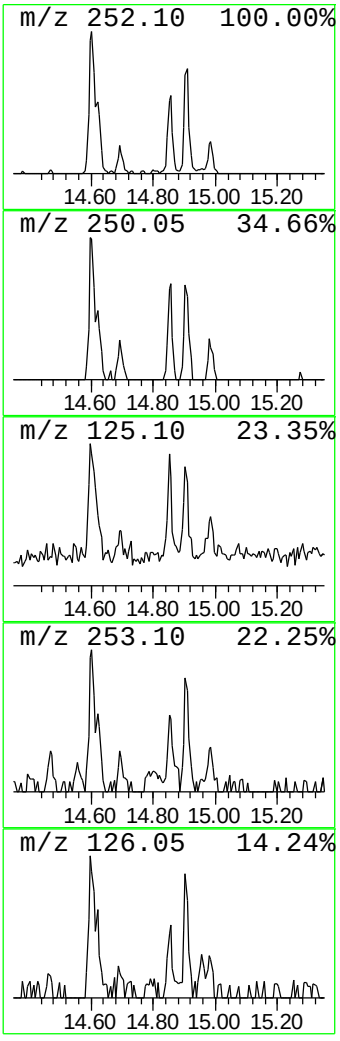
Peak Number 8 Perylene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.85	2.87 ng	41080	Perylene-d12	14.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Perylene	252	C20H12	000198-55-0	89
2	Benzo[a]pyrene	252	C20H12	000050-32-8	70
3	Benzo[j]fluoranthene	252	C20H12	000205-82-3	70
4	Benzo[e]pyrene	252	C20H12	000192-97-2	70
5	Benzo[k]fluoranthene	252	C20H12	000207-08-9	64





Data Path : Z:\HPCHEM1\BNA F\DATA\BF072717\
Data File : BF097139.D
Acq On : 27 Jul 2017 23:01
Operator : SJ/JU
Sample : I4424-10 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AU-06-072417-D

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.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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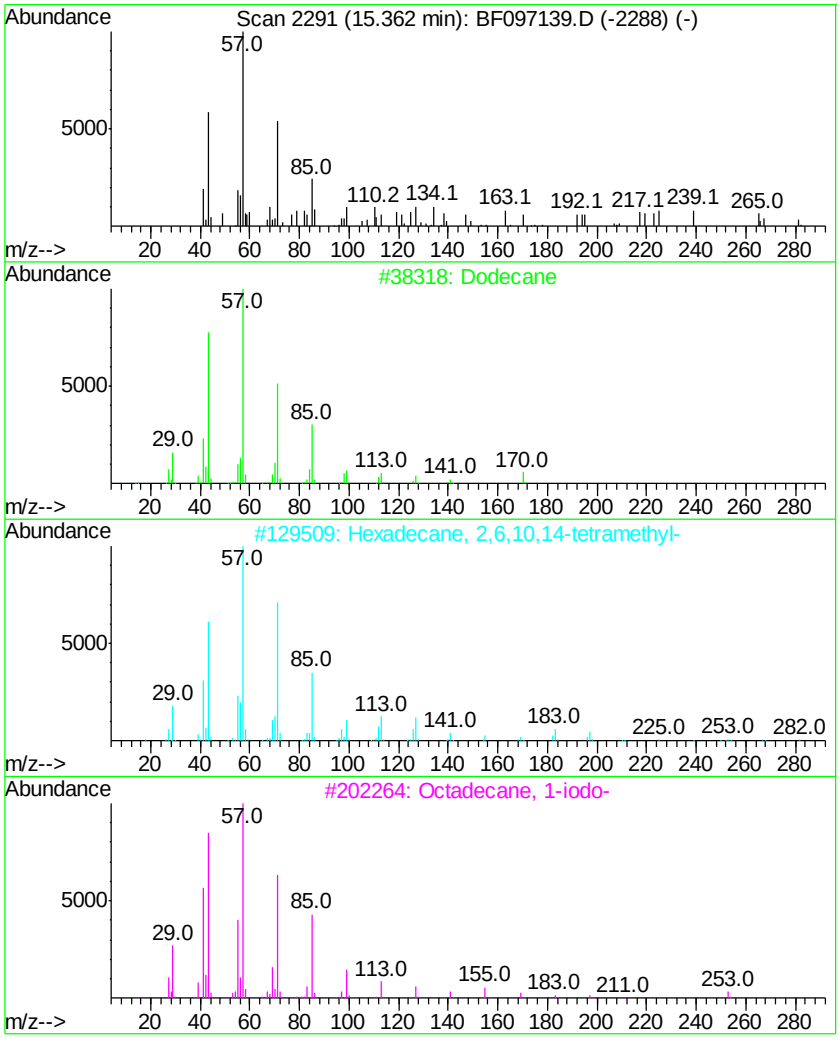
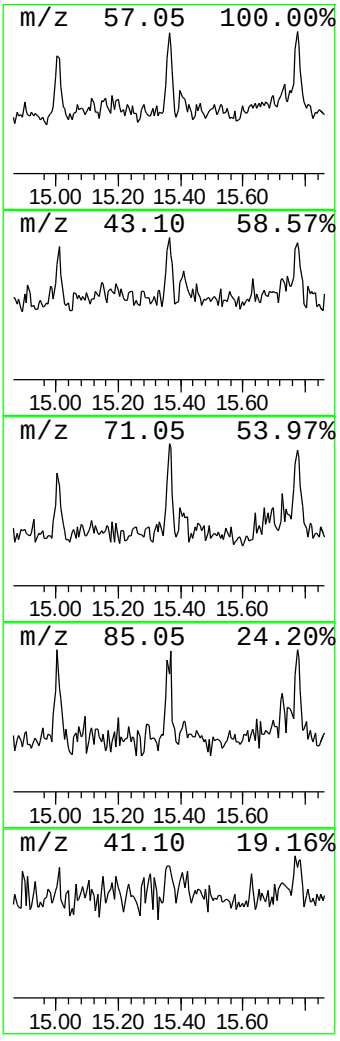
Peak Number 9 Dodecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.36	2.60 ng	37185	Perylene-d12	14.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane	170	C12H26	000112-40-3	52
2	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	50
3	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	47
4	Nonadecane, 4-methyl-	282	C20H42	025117-27-5	47
5	Docosane	310	C22H46	000629-97-0	47





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Data File : BF097139.D
Acq On : 27 Jul 2017 23:01
Operator : SJ/JU
Sample : I4424-10 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AU-06-072417-D

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

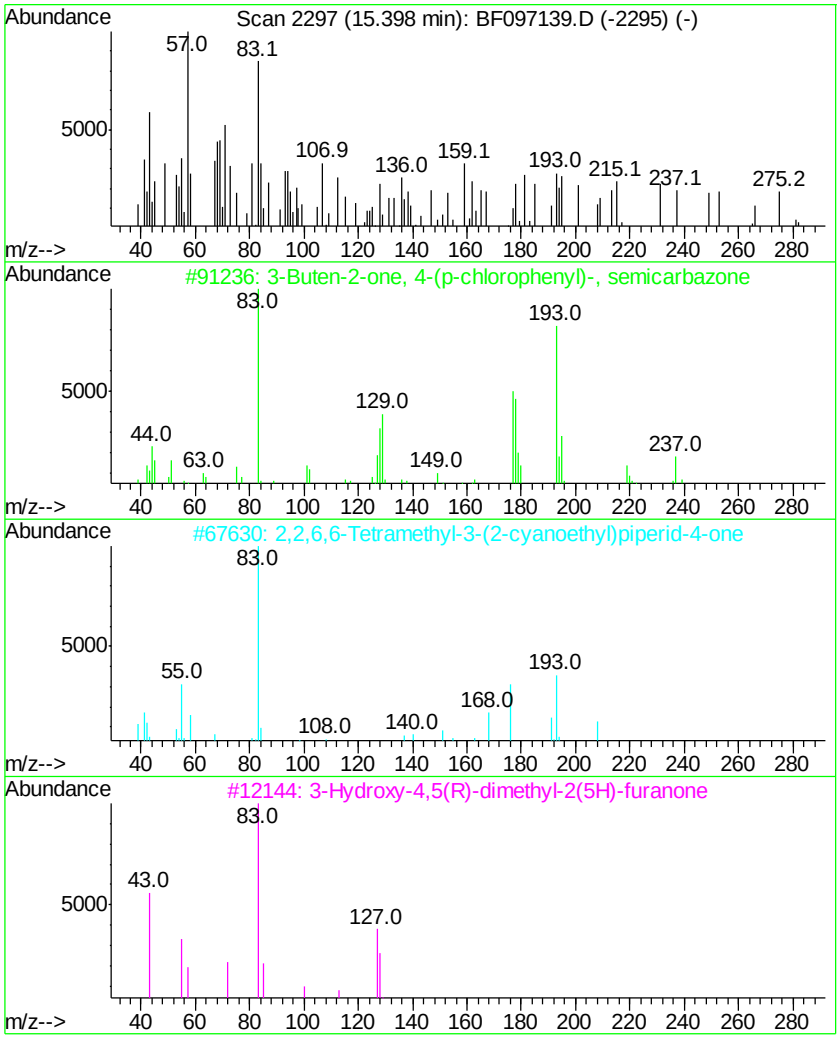
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

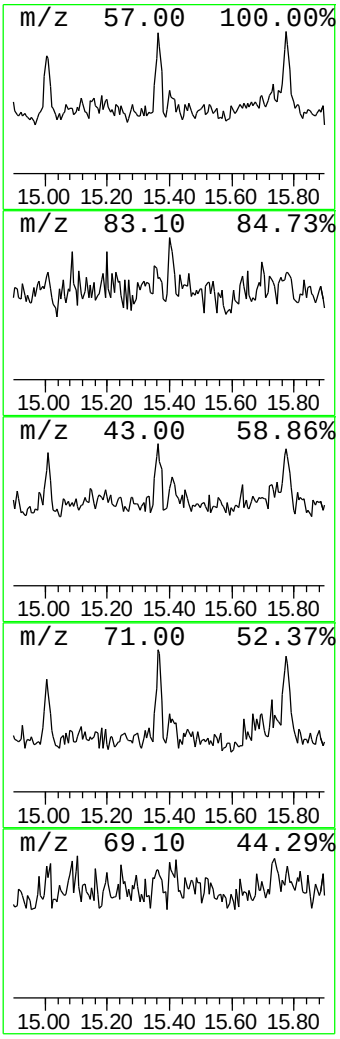
****

Peak Number 10 unknown15.40 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.40	3.34 ng	47849	Perylene-d12	14.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Buten-2-one, 4-(p-chlorophenyl...	237	C11H12ClN3O	017026-15-2	27
2	2,2,6,6-Tetramethyl-3-(2-cyanoet...	208	C12H20N2O	111335-32-1	22
3	3-Hydroxy-4,5(R)-dimethyl-2(5H)-...	128	C6H8O3	087068-70-0	14
4	1,1'-Bicyclohexyl, 2-(1-methylet...	208	C15H28	050991-15-6	14
5	Cyclohexane, (3-cyclopentylpropyl)-	194	C14H26	002883-07-0	12





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072717\
Data File : BF097139.D
Acq On : 27 Jul 2017 23:01
Operator : SJ/JU
Sample : I4424-10 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AU-06-072417-D

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

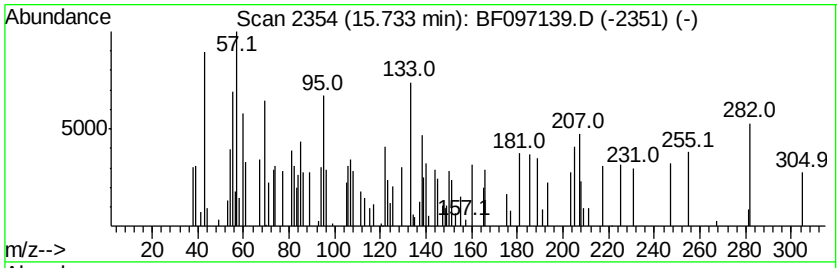
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

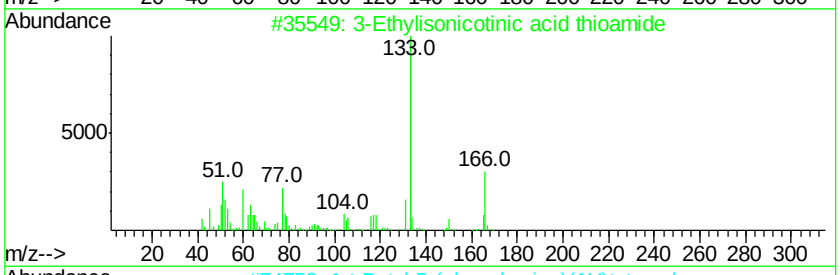
****

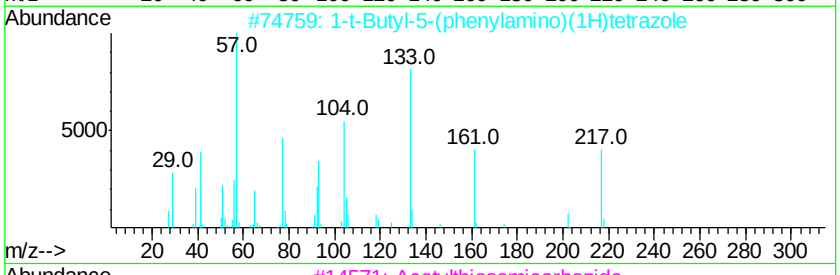
Peak Number 11 unknown15.73 Concentration Rank 11

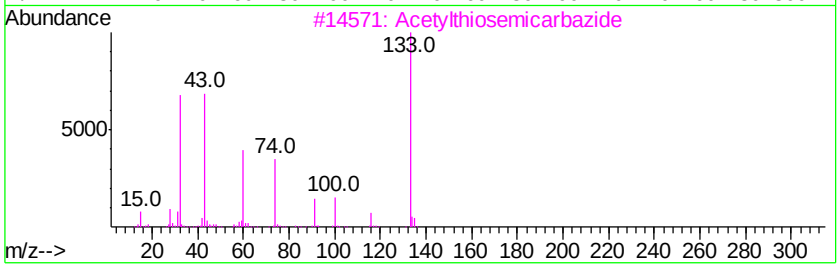
R.T.	EstConc	Area	Relative to ISTD	R.T.
15.73	2.11 ng	30168	Perylene-d12	14.96

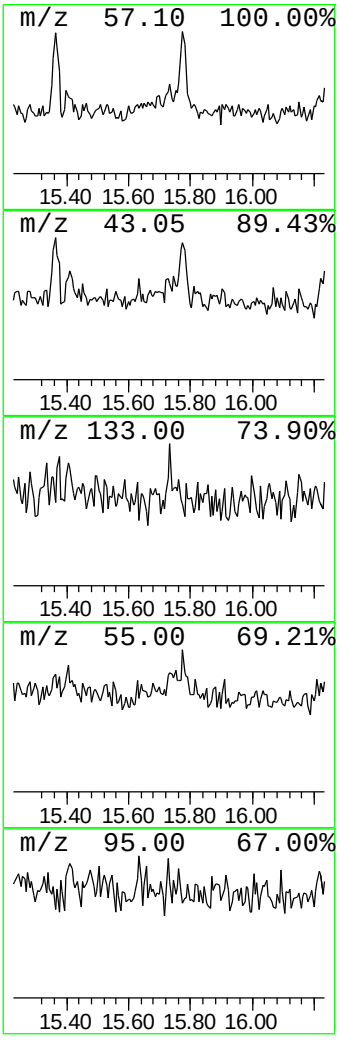
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Ethylisonicotinic acid thioamide	166	C8H10N2S	010605-12-6	11
2	1-t-Butyl-5-(phenylamino)(1H)tet...	217	C11H15N5	073027-67-5	10
3	Acetylthiosemicarbazide	133	C3H7N3OS	002302-88-7	10
4	Benzeneacetonitrile, 4-hydroxy-	133	C8H7NO	014191-95-8	10
5	1,3,4-Thiadiazol-2-amine, 5-(pro...	175	C5H9N3S2	030062-49-8	9











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Sample : I4424-10 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AU-06-072417-D

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.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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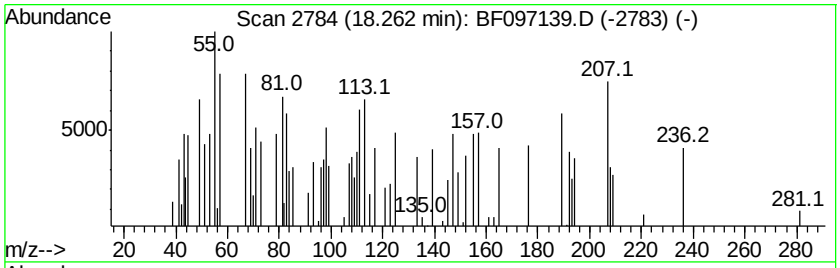
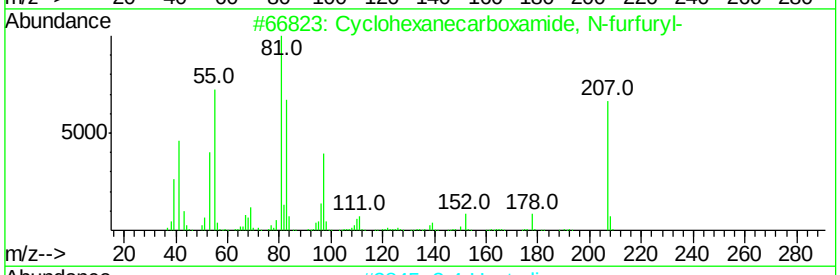
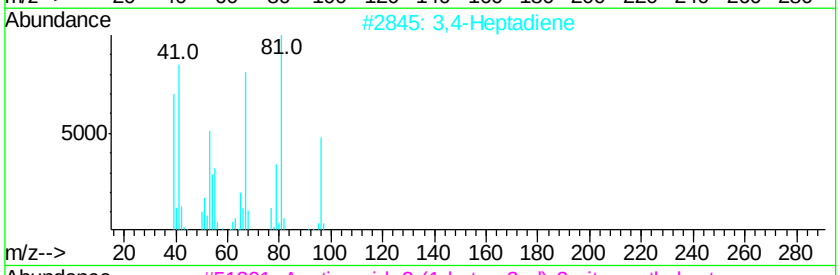
Peak Number 12 unknown18.26 Concentration Rank 10

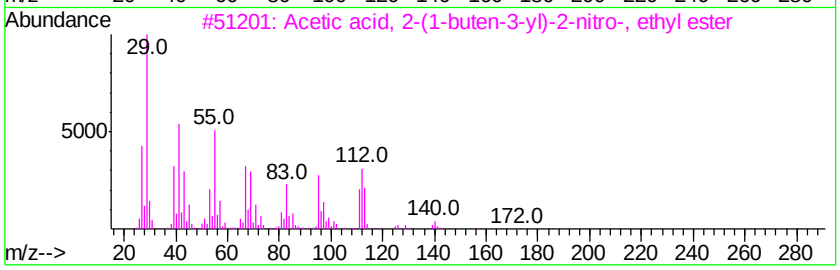
R.T.	EstConc	Area	Relative to ISTD	R.T.
18.26	2.13 ng	30518	Perylene-d12	14.96

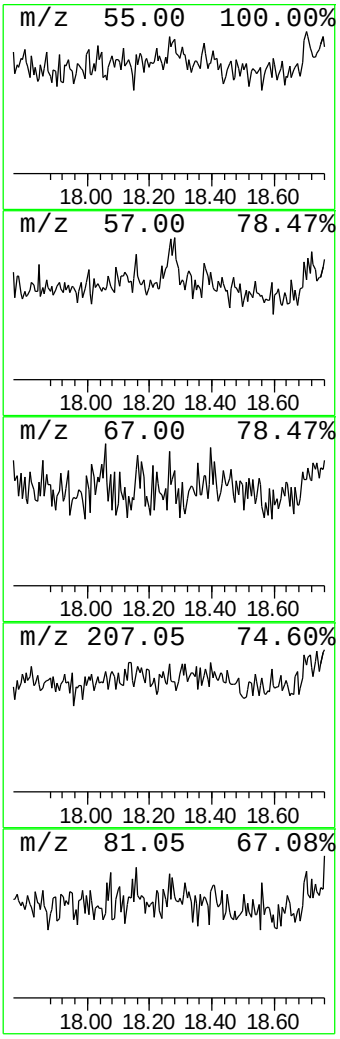
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanecarboxamide, N-furfuryl-	207	C12H17NO2	006341-32-8	25
2	3,4-Heptadiene	96	C7H12	002454-31-1	10
3	Acetic acid, 2-(1-buten-3-yl)-2-...	187	C8H13NO4	1000159-09-9	10
4	Cyclopropane, 1,1-dichloro-3-(1,...	194	C9H16Cl2	017171-92-5	10
5	4-Octyne	110	C8H14	001942-45-6	9











Data Path : Z:\HPCHEM1\BNA F\DATA\BF072717\
Data File : BF097139.D
Acq On : 27 Jul 2017 23:01
Operator : SJ/JU
Sample : I4424-10 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AU-06-072417-D

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.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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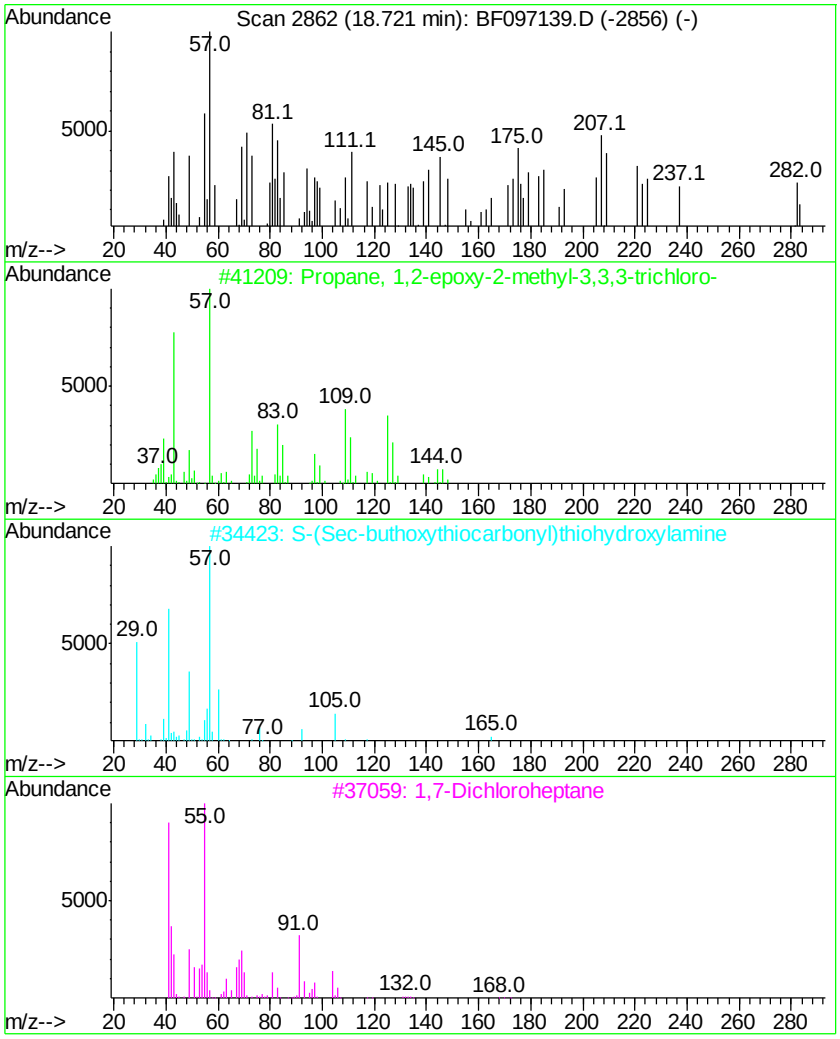
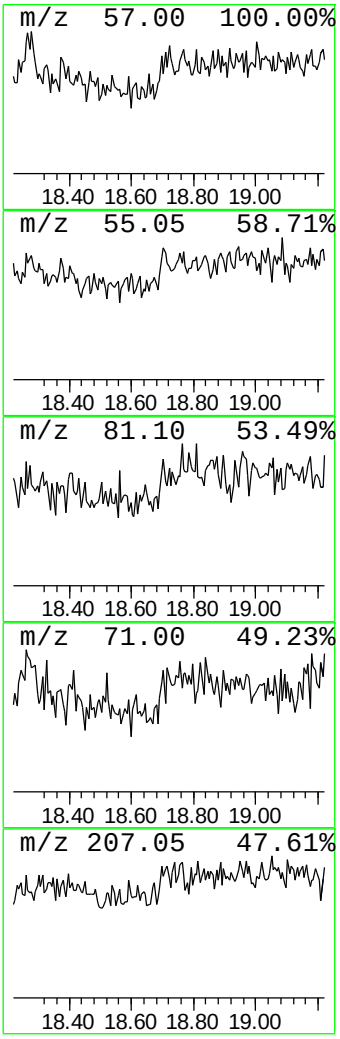
Peak Number 13 unknown18.72 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.72	3.02 ng	43141	Perylene-d12	14.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,2-epoxy-2-methyl-3,3,...	174	C4H5Cl3O	016387-26-1	10
2	S-(Sec-buthoxythiocarbonyl)thioh...	165	C5H11NOS2	035659-83-7	9
3	1,7-Dichloroheptane	168	C7H14Cl2	000821-76-1	9
4	1,1,3,3,5,5-Hexamethyl-1,5-bis(2...	352	C14H36O4Si3	1000364-61-1	9
5	Phosphine, cyclohexyl(1,1-dimeth...	186	C11H23P	074685-81-7	7





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072717\
Data File : BF097139.D
Acq On : 27 Jul 2017 23:01
Operator : SJ/JU
Sample : I4424-10 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AU-06-072417-D

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.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...	4.62	10.2	ng	187122	1	6.49	367475	20.0
unknown6.26	6.26	70.8	ng	1300980	1	6.49	367475	20.0
Pentadecane	10.44	3.0	ng	49870	4	10.99	334029	20.0
Pentafluoropropio...	13.48	2.0	ng	43965	5	13.61	430421	20.0
unknown14.41	14.41	3.4	ng	49119	6	14.96	286148	20.0
unknown14.69	14.69	2.0	ng	28644	6	14.96	286148	20.0
Perylene	14.85	2.9	ng	41080	6	14.96	286148	20.0
Dodecane	15.36	2.6	ng	37185	6	14.96	286148	20.0
unknown15.40	15.40	3.3	ng	47849	6	14.96	286148	20.0
unknown15.73	15.73	2.1	ng	30168	6	14.96	286148	20.0
unknown18.26	18.26	2.1	ng	30518	6	14.96	286148	20.0
unknown18.72	18.72	3.0	ng	43141	6	14.96	286148	20.0