LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF080817\
Data File : BF097488.D
Acq On : 9 Aug 2017 00:27
Operator : SJ/JU
Sample : I4657-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-01-080717-A

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	4.534	464	467	478	rBV	70608	134399	8.33%	0.806%
2	4.998	543	546	563	rBV	1194988	1585152	98.28%	9.501%
3	6.075	726	729	743	rBV	1464742	1612940	100.00%	9.667%
4	6.181	743	747	753	rVB	1413377	1490758	92.42%	8.935%
5	6.404	782	785	795	rBV	692930	642501	39.83%	3.851%
6	6.557	808	811	826	rBV	1134172	1087595	67.43%	6.519%
7	6.975	879	882	902	rBV	879044	909675	56.40%	5.452%
8	7.686	1000	1003	1013	rBV	943199	871912	54.06%	5.226%
9	8.763	1183	1186	1199	rBV	1524782	1420826	88.09%	8.516%
10	9.169	1252	1255	1264	rBV	336447	286512	17.76%	1.717%
11	9.392	1289	1293	1296	rBV	24508	21768	1.35%	0.130%
12	9.427	1296	1299	1304	rBV	785463	738175	45.77%	4.424%
13	9.886	1374	1377	1380	rVB	41131	32171	1.99%	0.193%
14	10.104	1409	1414	1417	rBV	16072	22378	1.39%	0.134%
15	10.216	1430	1433	1441	rBV	728110	751549	46.59%	4.504%
16	10.357	1453	1457	1466	rBV	45433	54908	3.40%	0.329%
17	10.804	1529	1533	1535	rBV3	29352	30445	1.89%	0.182%
18	10.904	1547	1550	1553	rBV	684085	605322	37.53%	3.628%
19	10.927	1553	1554	1560	rVB	61391	43642	2.71%	0.262%
20	10.986	1561	1564	1569	rVB	20630	19396	1.20%	0.116%
21	11.410	1631	1636	1638	rBV2	25369	25359	1.57%	0.152%
22	11.463	1643	1645	1648	rVV2	46181	53600	3.32%	0.321%
23	11.516	1651	1654	1657	rVV	52609	62496	3.87%	0.375%
24	11.539	1657	1658	1664	rVB2	20822	18708	1.16%	0.112%
25	11.957	1725	1729	1731	rBV	32863	33203	2.06%	0.199%
26	12.051	1741	1745	1748	rBV3	19837	29202	1.81%	0.175%
27	12.110	1752	1755	1760	rBV	156722	149529	9.27%	0.896%
28	12.163	1761	1764	1770	rVV6	10244	19759	1.23%	0.118%
29	12.333	1788	1793	1796	rBV	172403	170563	10.57%	1.022%
30	12.486	1815	1819	1826	rVB	1027386	950385	58.92%	5.696%
31	12.557	1828	1831	1834	rBV3	19453	24562	1.52%	0.147%
32	12.651	1844	1847	1848	rBV3	18155	18450	1.14%	0.111%
33	12.668	1848	1850	1855	rVB	33051	33380	2.07%	0.200%
34	12.733	1857	1861	1863	rBV3	33353	32420	2.01%	0.194%

LSC Area Percent Report

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Acq On : 9 Aug 2017 00:27
Operator : SJ/JU
Sample : I4657-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-01-080717-A

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	12.768	1865	1867	1871	rVB2	21804	28600	1.77%	0.171%
36	12.863	1880	1883	1886	rBV2	34664	34444	2.14%	0.206%
37	12.892	1886	1888	1891	rVV2	18125	19461	1.21%	0.117%
38	13.527	1992	1996	1999	rBV	609106	611301	37.90%	3.664%
39	13.557	1999	2001	2007	rVB	70222	73020	4.53%	0.438%
40	13.768	2036	2037	2039	rBV2	25597	16402	1.02%	0.098%
41	13.880	2054	2056	2060	rBV3	46545	48043	2.98%	0.288%
42	13.921	2060	2063	2066	rVB3	37362	36491	2.26%	0.219%
43	13.957	2066	2069	2072	rBV4	40675	52876	3.28%	0.317%
44	14.374	2137	2140	2147	rBV	89805	108263	6.71%	0.649%
45	14.439	2147	2151	2155	rBV7	43907	104059	6.45%	0.624%
46	14.633	2181	2184	2191	rBV8	47899	102490	6.35%	0.614%
47	14.768	2205	2207	2210	rBV	57102	59307	3.68%	0.355%
48	14.821	2213	2216	2220	rVV	74403	109373	6.78%	0.656%
49	14.868	2220	2224	2229	rVB	421265	457646	28.37%	2.743%
50	14.962	2236	2240	2244	rVB7	49317	88557	5.49%	0.531%
51	15.009	2246	2248	2249	rBV2	36816	33581	2.08%	0.201%
52	15.403	2313	2315	2320	rBV5	47798	68996	4.28%	0.414%
53	15.739	2367	2372	2375	rBV7	47536	90412	5.61%	0.542%
54	15.827	2382	2387	2391	rBV7	38877	92505	5.74%	0.554%
55	16.139	2438	2440	2446	rBV7	28716	53997	3.35%	0.324%
56	16.198	2448	2450	2454	rBV5	28765	39576	2.45%	0.237%
57	16.339	2472	2474	2477	rBV4	36467	49819	3.09%	0.299%
58	16.962	2578	2580	2581	rBV	26850	18006	1.12%	0.108%
59	17.262	2627	2631	2633	rBV5	33243	52885	3.28%	0.317%
60	17.492	2665	2670	2672	rBV6	28886	52768	3.27%	0.316%
61	18.444	2830	2832	2836	rBV4	17039	19041	1.18%	0.114%
62	18.509	2840	2843	2850	rVB8	22829	51672	3.20%	0.310%
63	18.633	2861	2864	2869	rBV6	23075	44543	2.76%	0.267%
64	18.686	2871	2873	2876	rBV4	14492	19163	1.19%	0.115%
65	18.833	2894	2898	2902	rBV7	18210	38105	2.36%	0.228%
66	19.121	2944	2947	2949	rBV3	21224	25639	1.59%	0.154%

Sum of corrected areas: 16684681

LSC Report - Integrated Chromatogram

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Data File : BF097488.D
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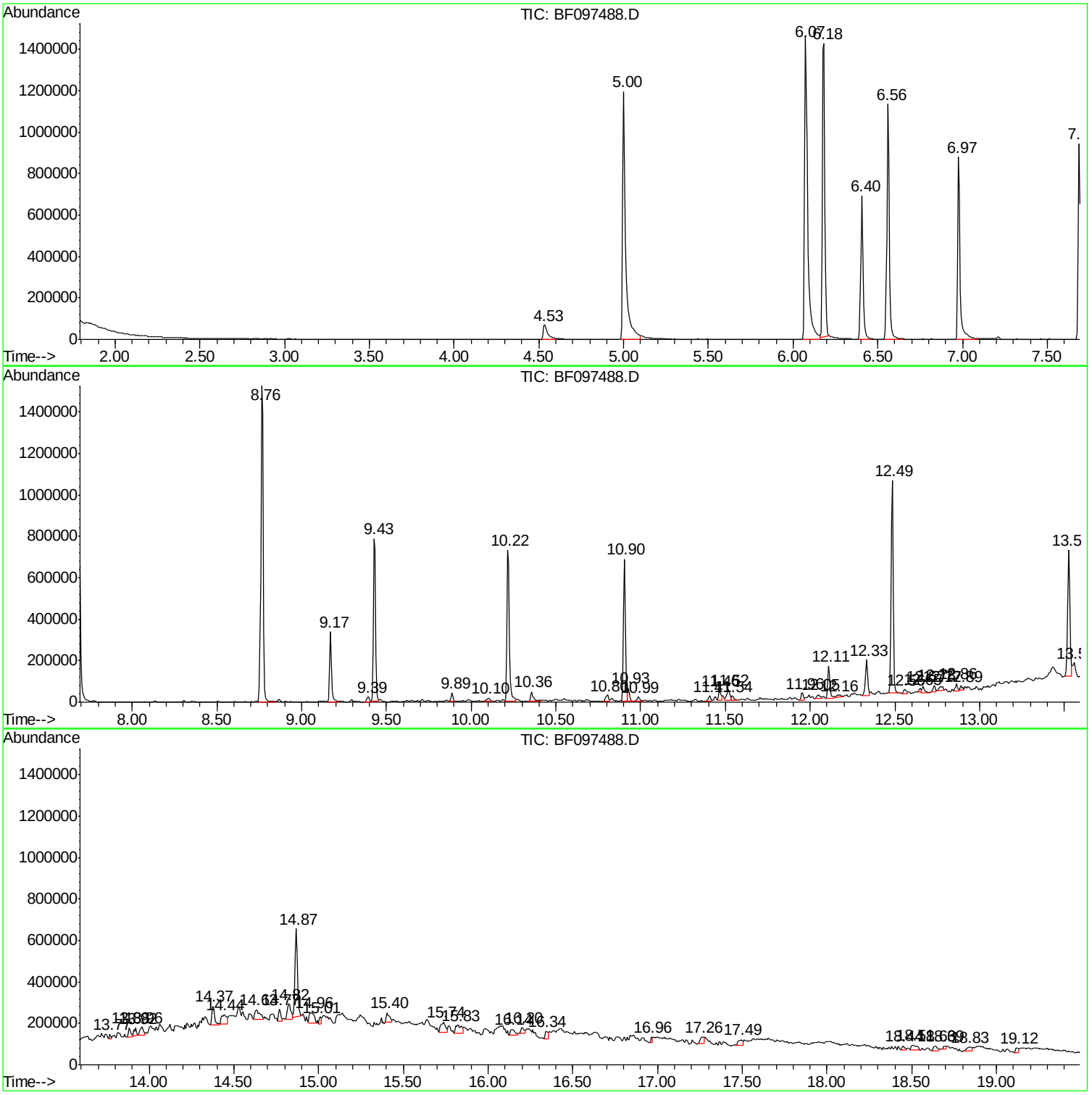
Operator : SJ/JU
Sample : I4657-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-01-080717-A

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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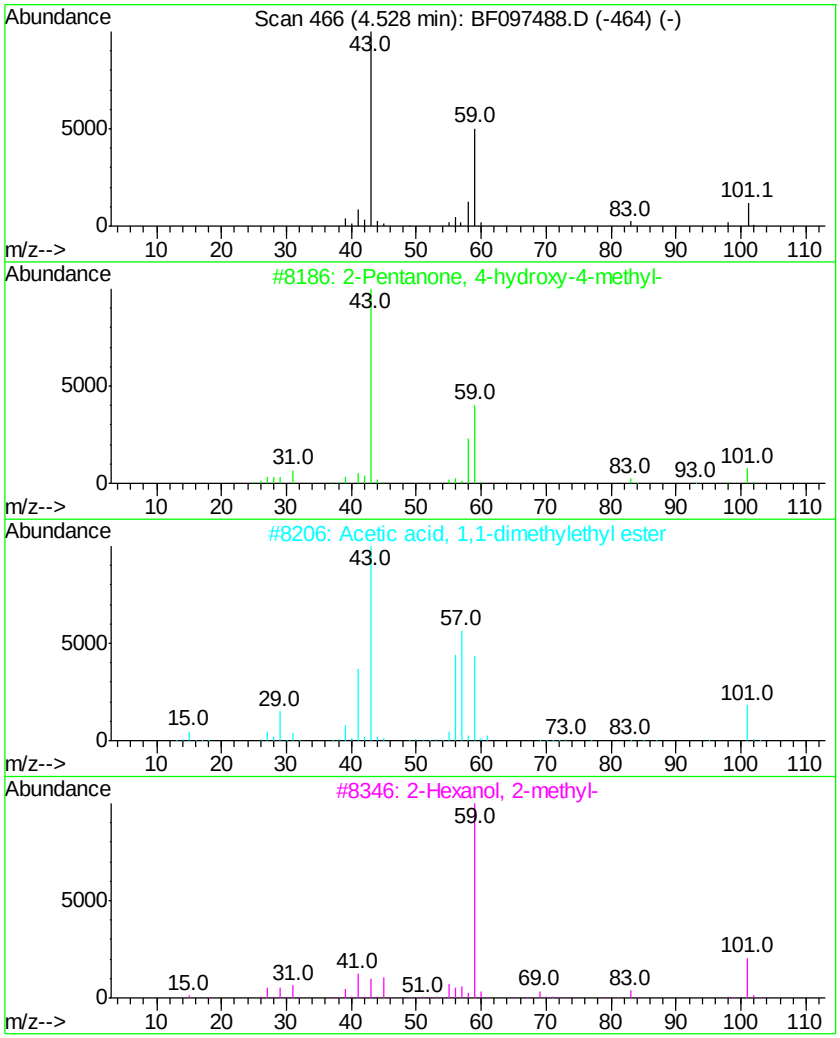
TIC Integration Parameters: LSCINT.P

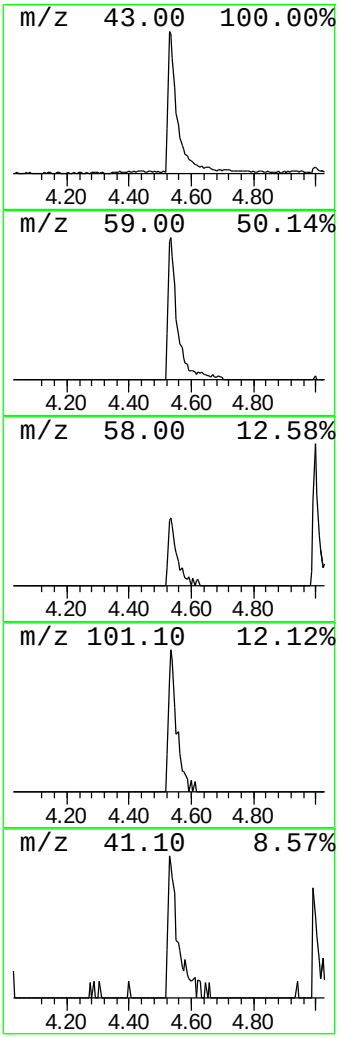
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.53	4.18 ng	134399	1,4-Dichlorobenzene-d4	6.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16





Data Path : Z:\HPCHEM1\BNA F\DATA\BF080817\
Data File : BF097488.D
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Operator : SJ/JU
Sample : I4657-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-01-080717-A

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

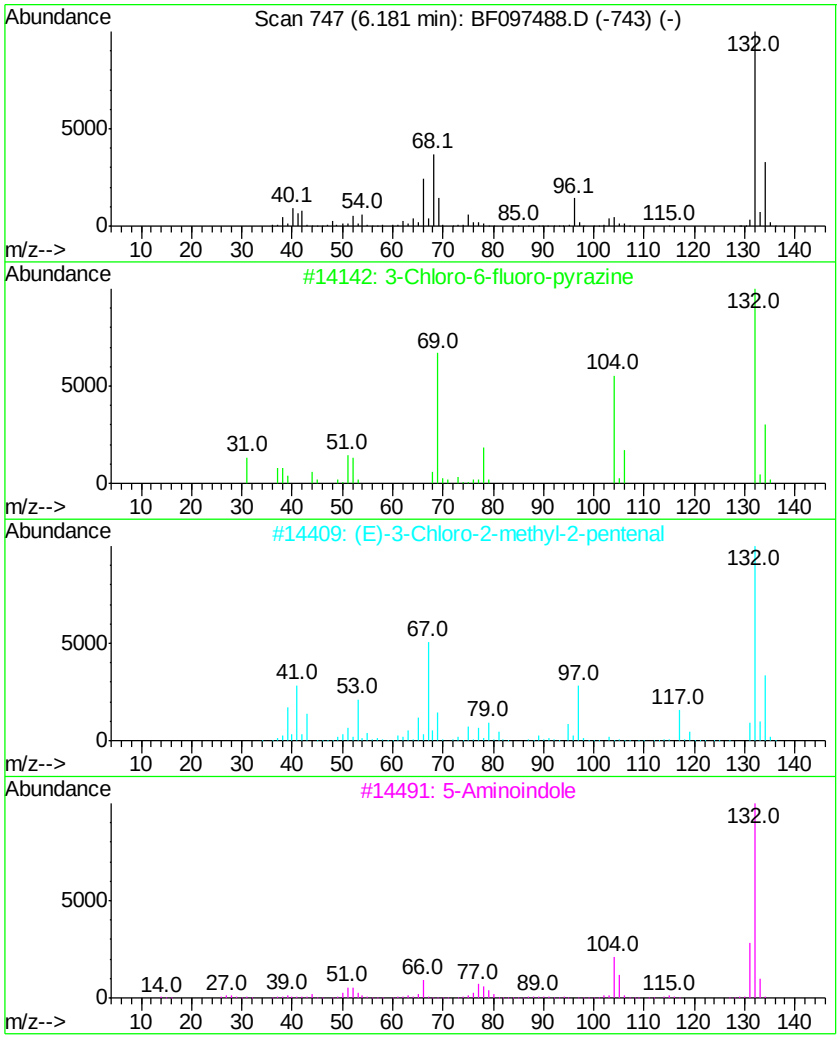
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

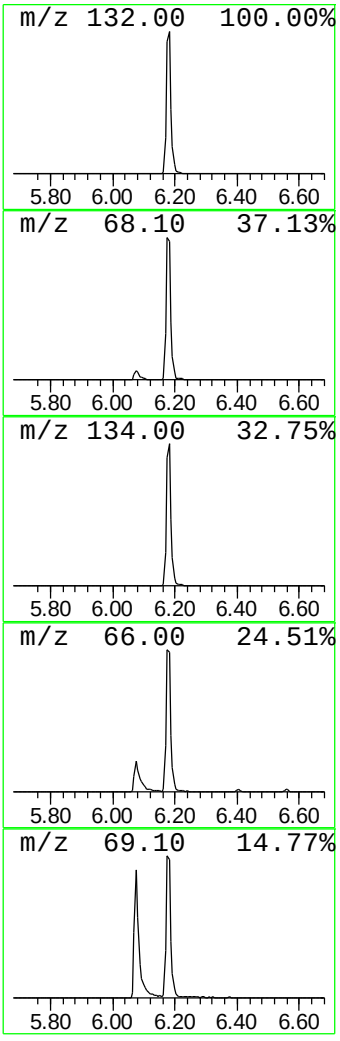
****

Peak Number 2 unknown6.18 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.18	46.40 ng	1490760	1,4-Dichlorobenzene-d4	6.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





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Sample : I4657-01
Misc :
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Instrument : BNA_F
ClientSampleId : CL-01-080717-A

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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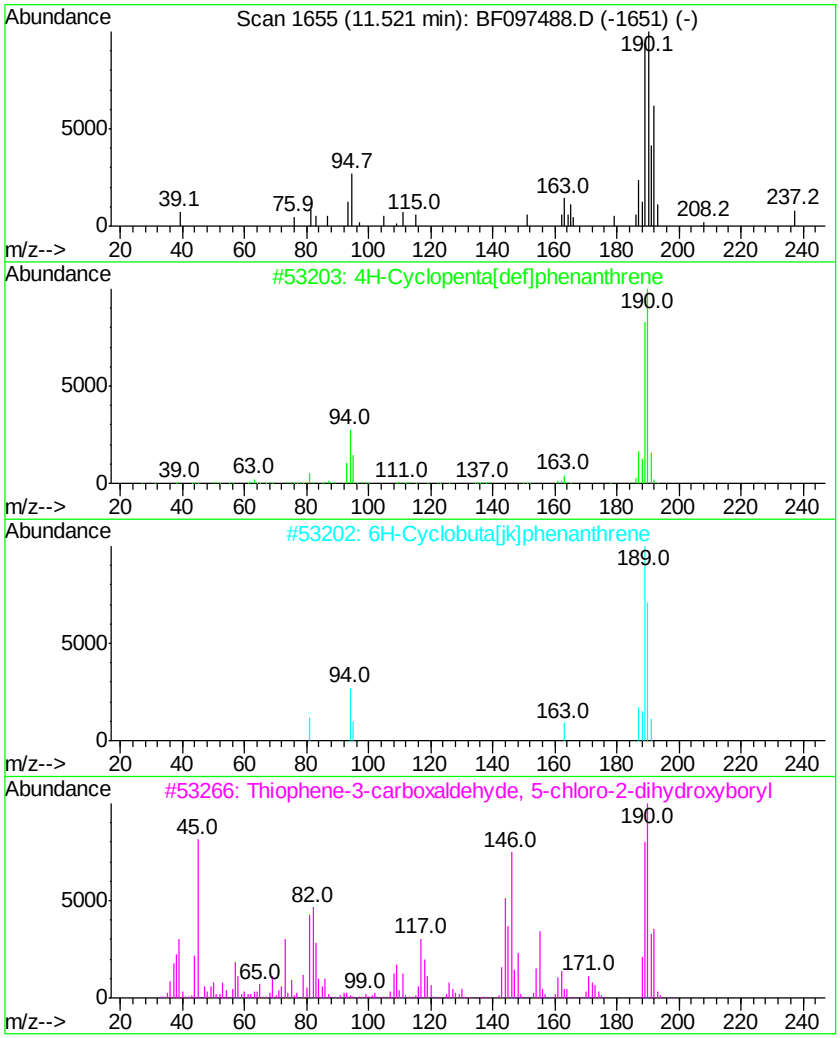
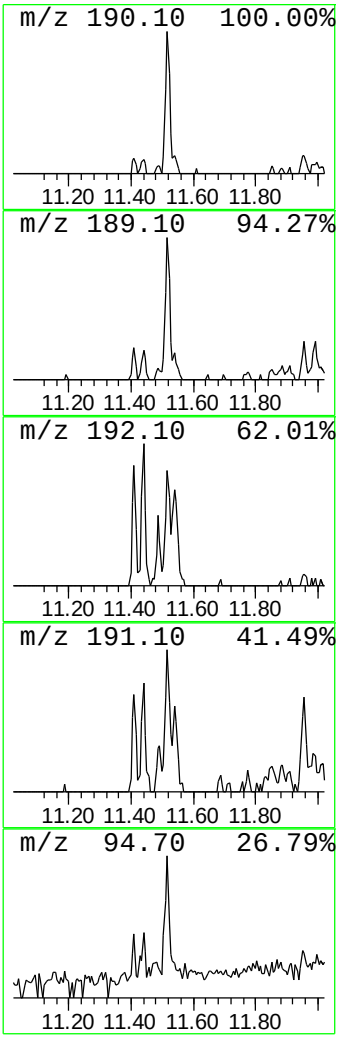
Peak Number 4 4H-Cyclopenta[def]phenanthrene Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.52	2.06 ng	62496	Phenanthrene-d10	10.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	64
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	58
3	Thiophene-3-carboxaldehyde, 5-ch...	190	C5H4BClO3S	036155-87-0	40
4	Methyl diselenide	190	C2H6Se2	007101-31-7	27
5	2,6-Dichlorobenzaldoxime	189	C7H5Cl2NO	025185-95-9	25





Data Path : Z:\HPCHEM1\BNA F\DATA\BF080817\
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Sample : I4657-01
Misc :
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Instrument : BNA_F
ClientSampleId : CL-01-080717-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
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TIC Library : C:\DATABASE\NIST11.L
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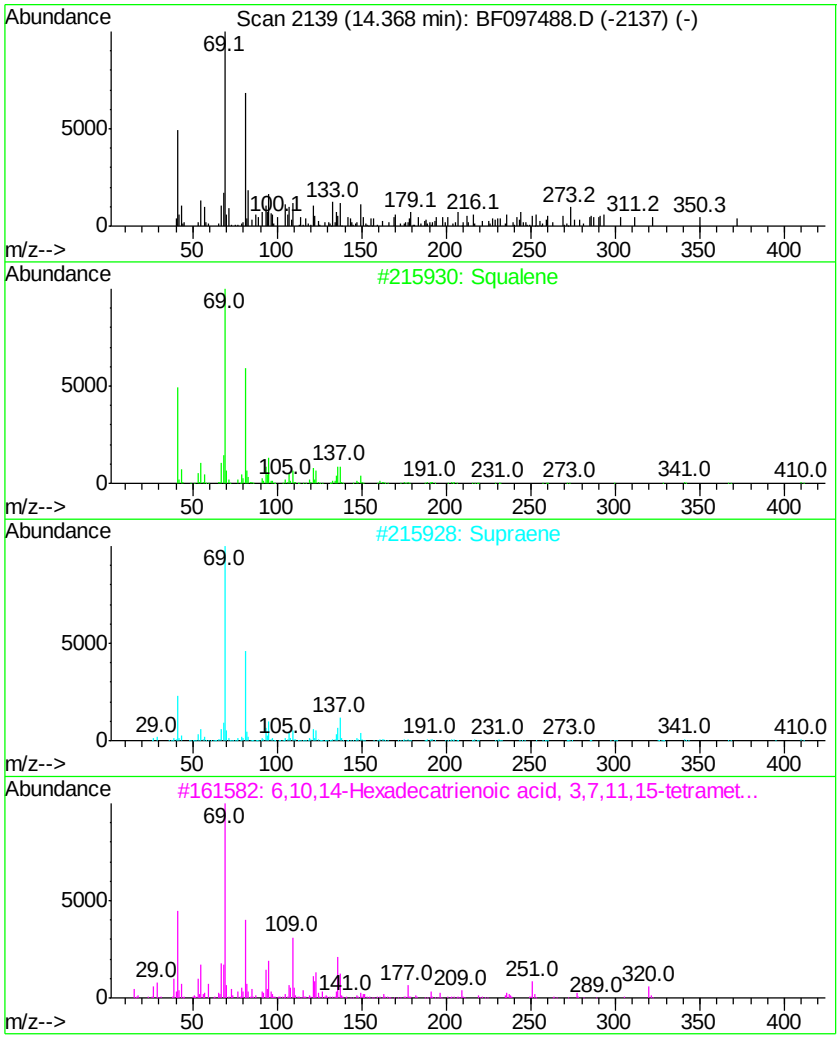
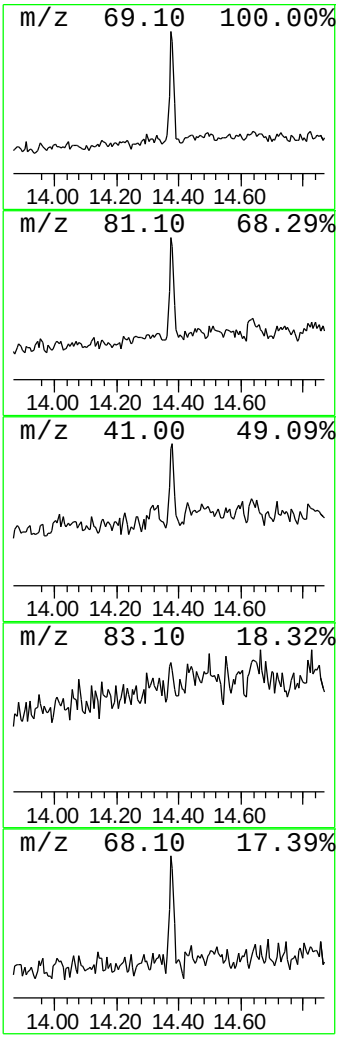
Peak Number 5 Squalene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.37	4.73 ng	108263	Perylene-d12	14.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	83
2	Supraene	410	C30H50	007683-64-9	80
3	6,10,14-Hexadecatrienoic acid, 3...	320	C21H36O2	036237-72-6	72
4	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	68
5	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64





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Data File : BF097488.D
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Sample : I4657-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-01-080717-A

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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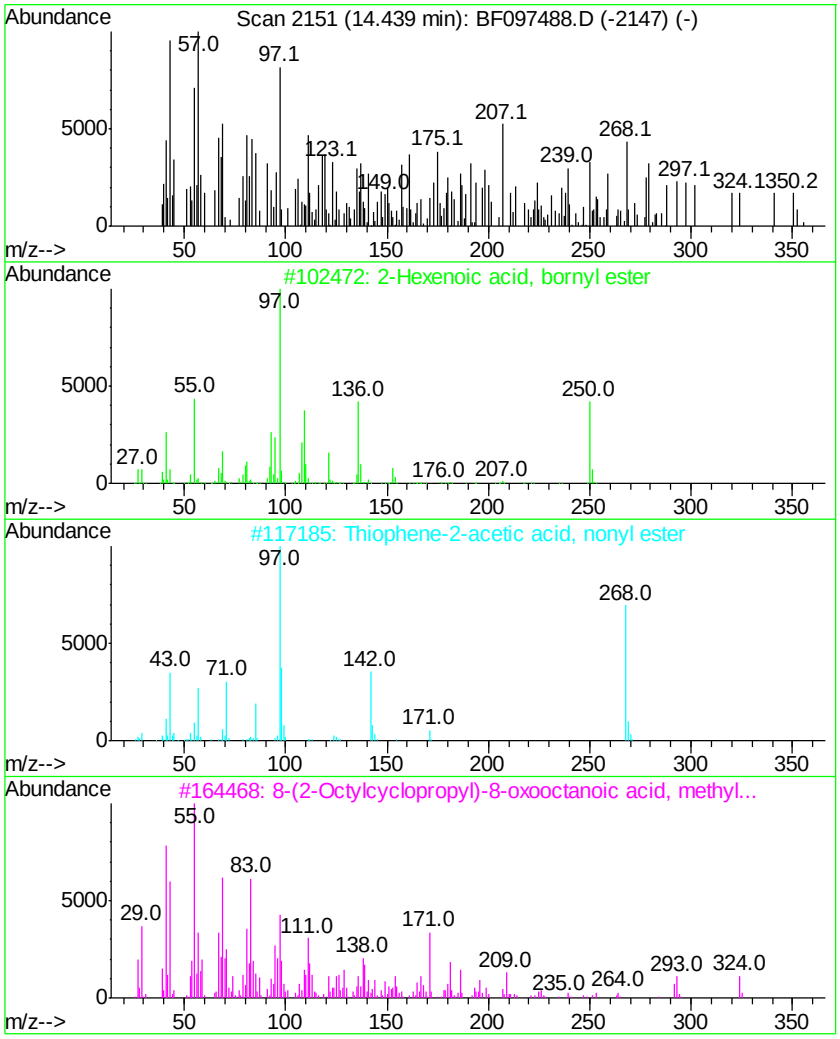
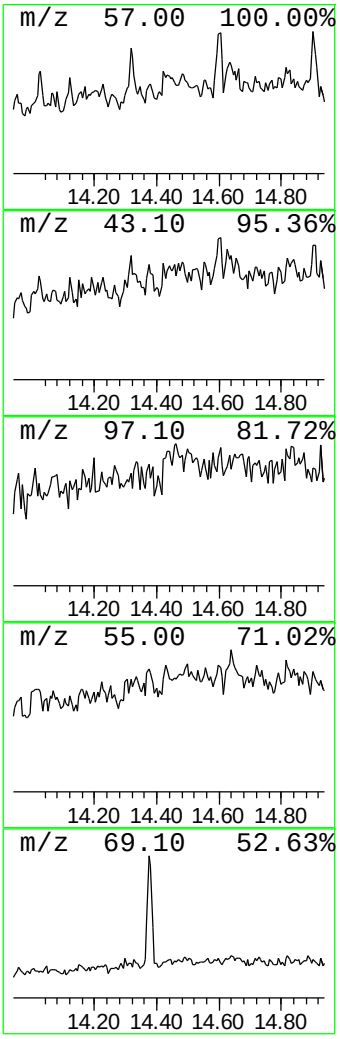
Peak Number 6 unknown14.44 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.44	4.55 ng	104059	Perylene-d12	14.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hexenoic acid, bornyl ester	250	C16H26O2	1000163-79-6	30
2	Thiophene-2-acetic acid, nonyl e...	268	C15H24O2S	1000282-82-3	27
3	8-(2-Octylcyclopropyl)-8-oxoocta...	324	C20H36O3	1000191-57-8	18
4	Hexadecanedinitrile	248	C16H28N2	006812-44-8	15
5	Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	004926-78-7	11





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Sample : I4657-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-01-080717-A

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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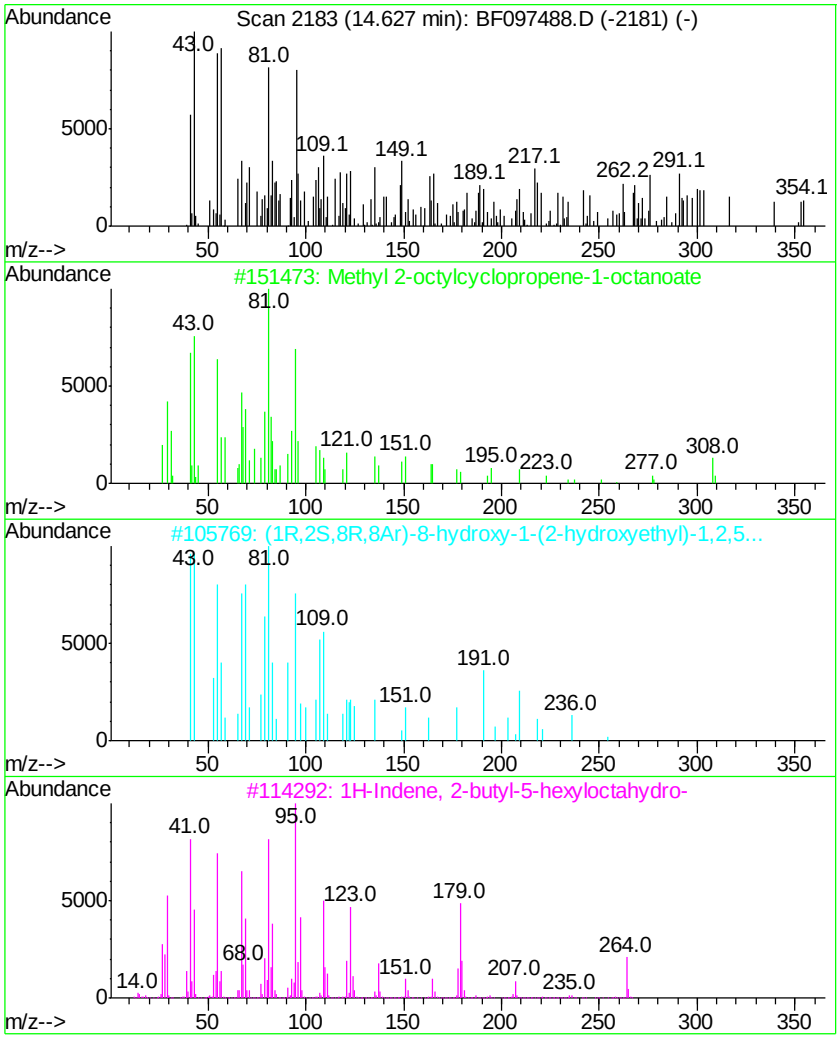
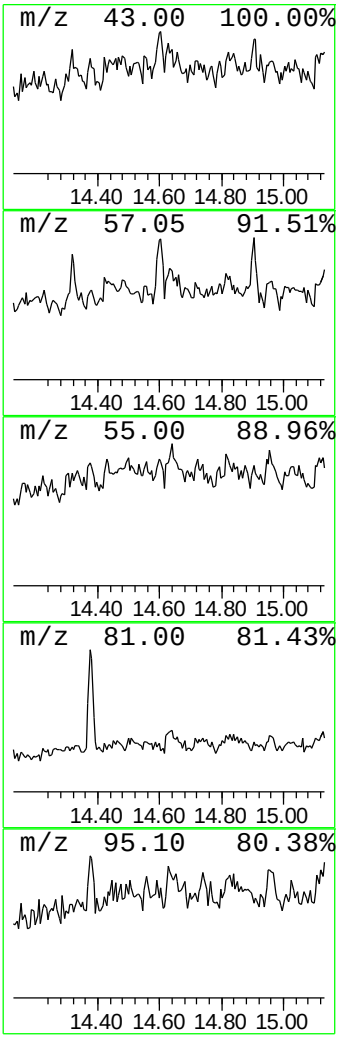
Peak Number 7 unknown14.63 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.63	4.48 ng	102490	Perylene-d12	14.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl 2-octylcyclopropene-1-oct...	308	C20H36O2	003220-60-8	43
2	(1R,2S,8R,8Ar)-8-hydroxy-1-(2-hy...	254	C16H30O2	1000298-98-3	43
3	1H-Indene, 2-butyl-5-hexyloctahy...	264	C19H36	055044-33-2	43
4	1,1'-Bicyclohexyl, 4-propoxy-4'-...	266	C18H34O	098321-58-5	38
5	Thioctic acid	206	C8H14O2S2	001077-28-7	38





Data Path : Z:\HPCHEM1\BNA F\DATA\BF080817\
Data File : BF097488.D
Acq On : 9 Aug 2017 00:27
Operator : SJ/JU
Sample : I4657-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-01-080717-A

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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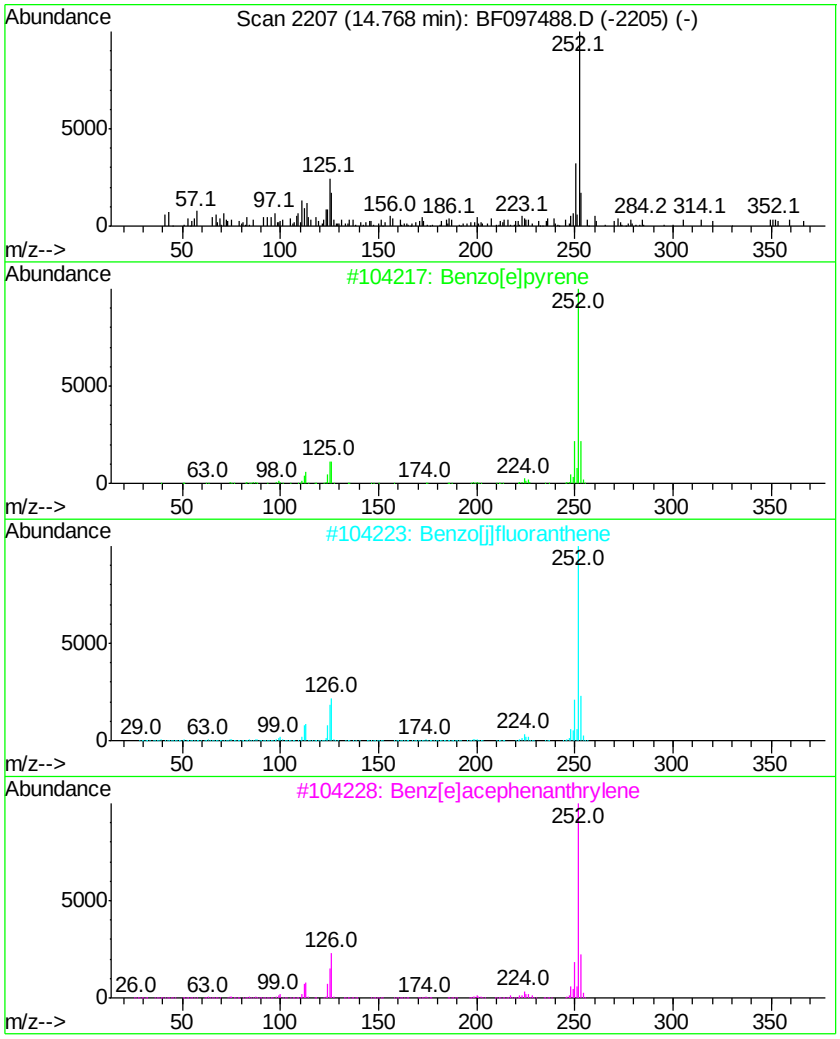
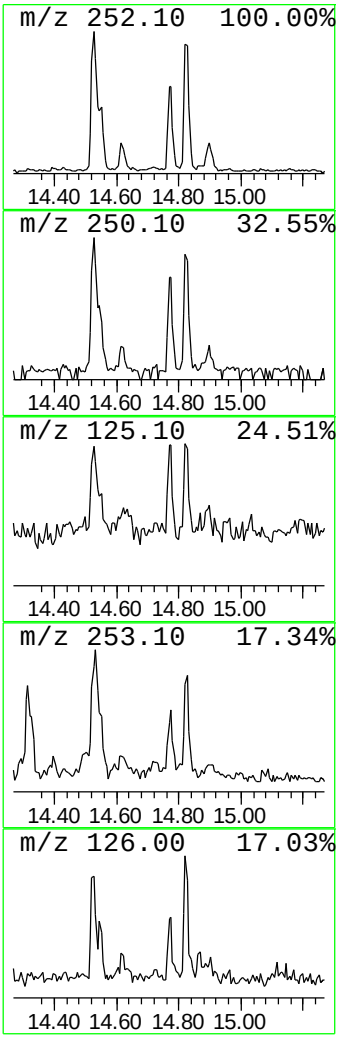
Peak Number 8 Benzo[e]pyrene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.77	2.59 ng	59307	Perylene-d12	14.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	93
2	Benzo[j]fluoranthene	252	C20H12	000205-82-3	92
3	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	92
4	Benzo[k]fluoranthene	252	C20H12	000207-08-9	86
5	Benzo[a]pyrene	252	C20H12	000050-32-8	83





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Data File : BF097488.D
Acq On : 9 Aug 2017 00:27
Operator : SJ/JU
Sample : I4657-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-01-080717-A

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

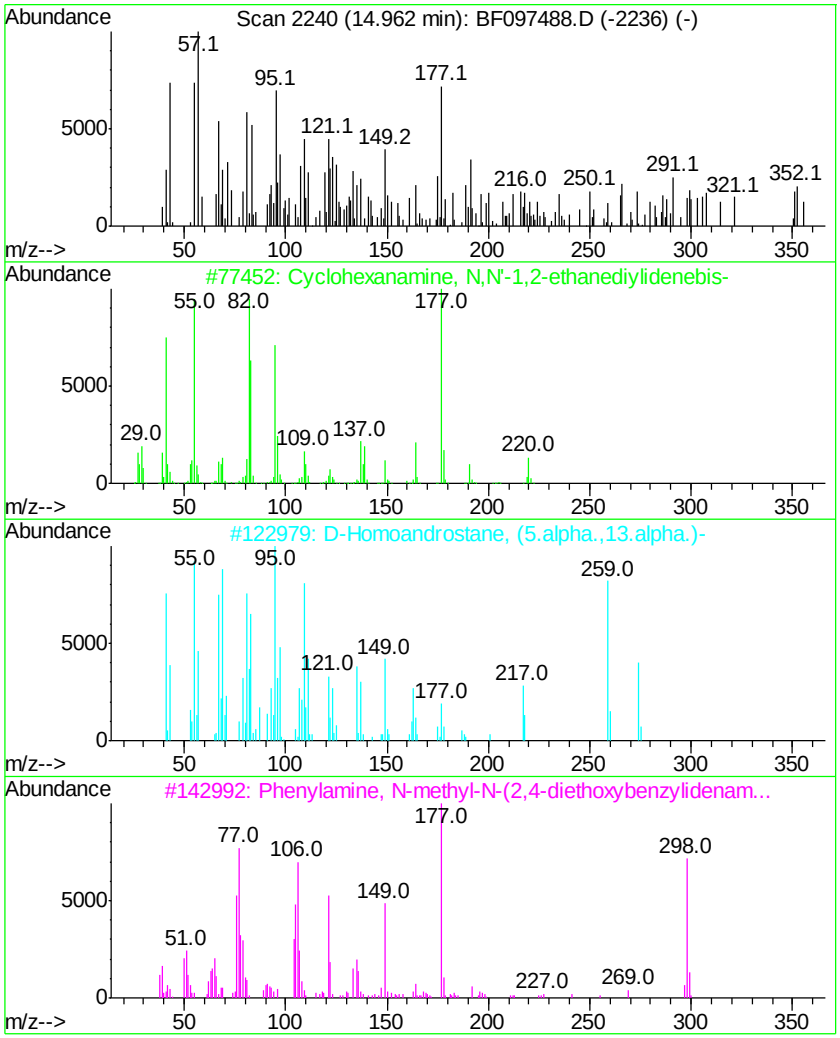
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

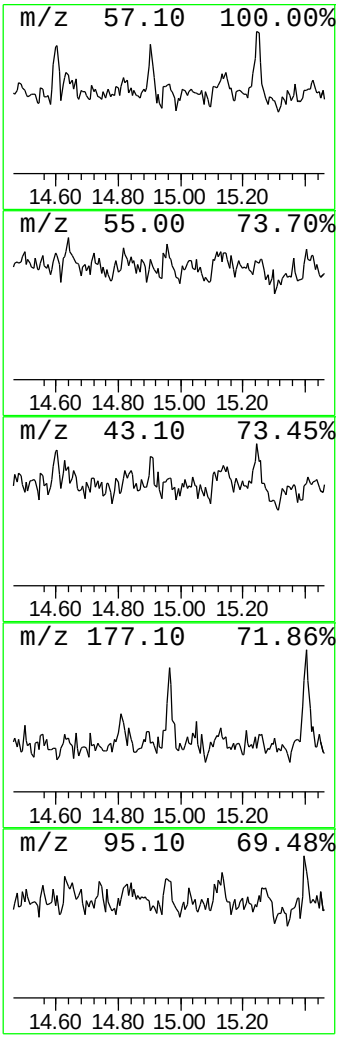
****

Peak Number 9 unknown14.96 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.96	3.87 ng	88557	Perylene-d12	14.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanamine, N,N'-1,2-ethane...	220	C14H24N2	003673-06-1	38
2	D-Homoandrostane, (5.alpha.,13.a...	274	C20H34	054482-31-4	27
3	Phenylamine, N-methyl-N-(2,4-die...	298	C18H22N2O2	1000223-55-3	18
4	4-Ethyl-2-hexynal	124	C8H12O	071932-97-3	18
5	8-Methyl-9,11-tridecadienol prop...	266	C17H30O2	1000130-96-9	18





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Acq On : 9 Aug 2017 00:27
Operator : SJ/JU
Sample : I4657-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-01-080717-A

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

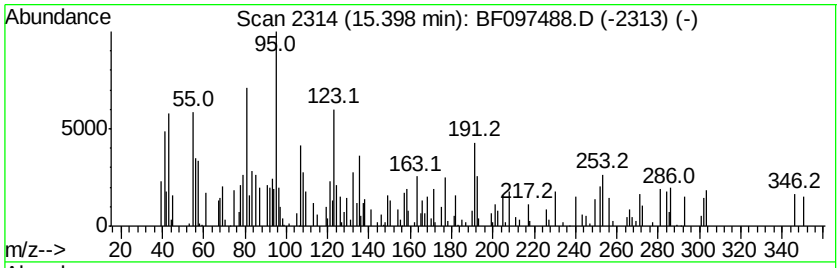
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

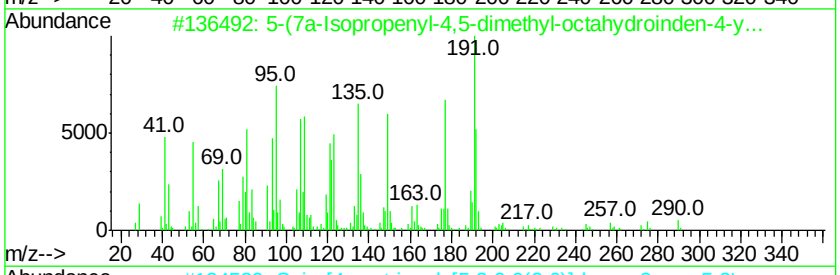
****

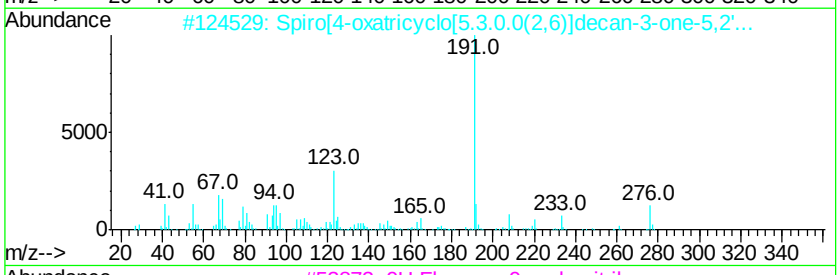
Peak Number 10 unknown15.40 Concentration Rank 10

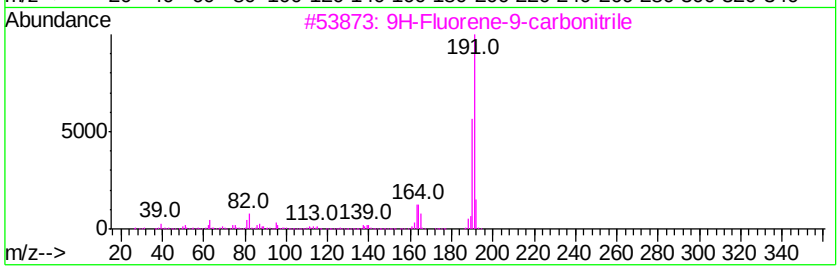
R.T.	EstConc	Area	Relative to ISTD	R.T.
15.40	3.02 ng	68996	Perylene-d12	14.87

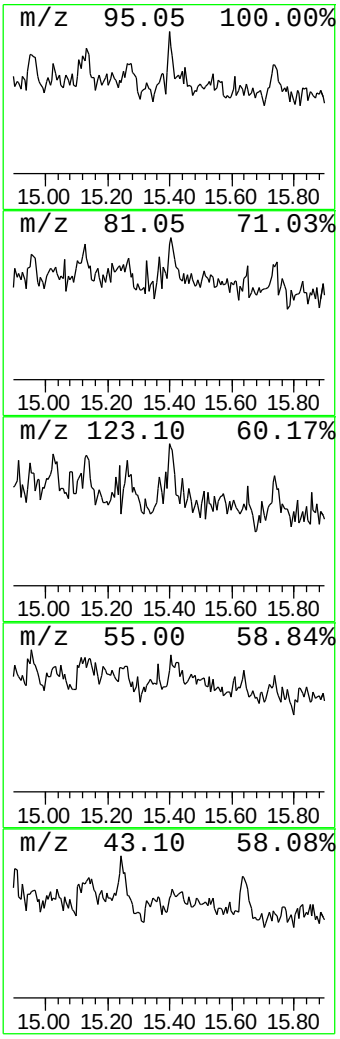
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-(7a-Isopropenyl-4,5-dimethyl-o...	290	C20H34O	1000193-54-0	38
2	Spiro[4-oxatricyclo[5.3.0.0(2,6)...	276	C18H28O2	1000156-82-9	35
3	9H-Fluorene-9-carbonitrile	191	C14H9N	001529-40-4	25
4	Thiazole, 2-amino-4-(p-aminophen...	191	C9H9N3S	003673-53-8	22
5	.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	22











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Data File : BF097488.D
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Operator : SJ/JU
Sample : I4657-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-01-080717-A

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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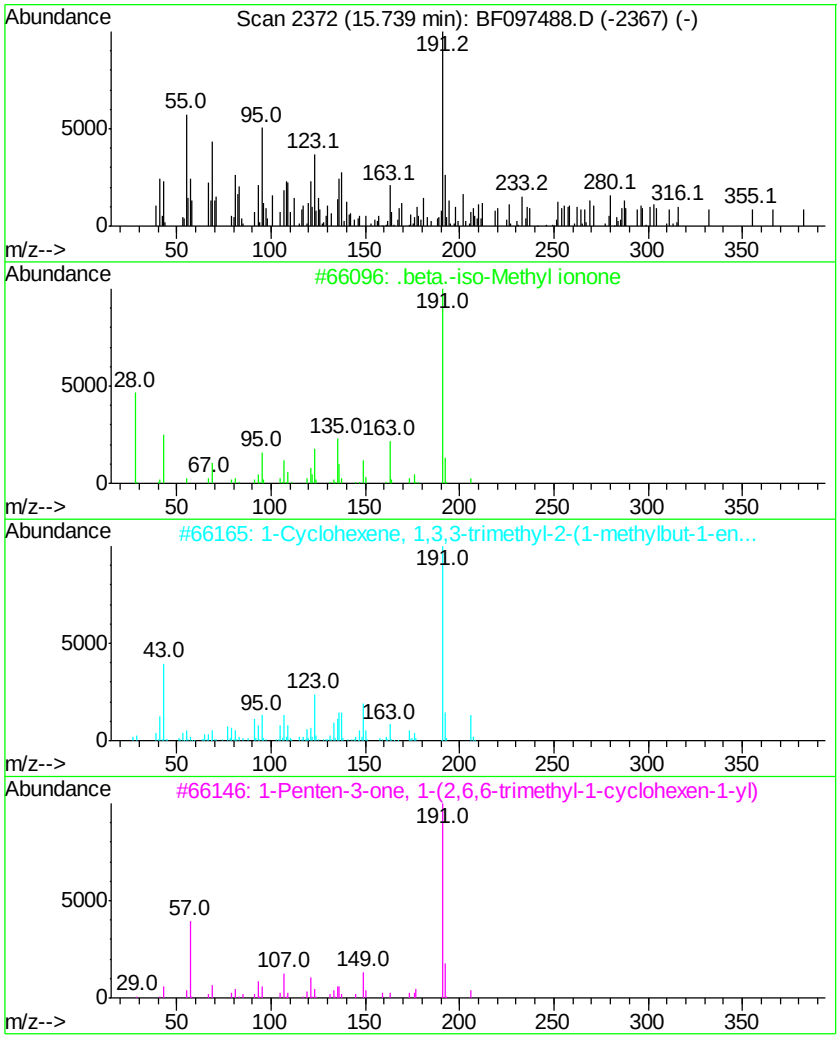
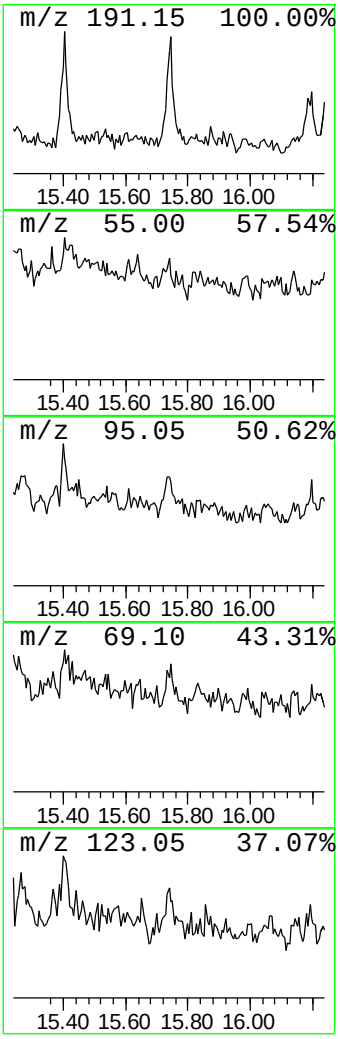
Peak Number 11 .beta.-iso-Methyl ionone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.74	3.95 ng	90412	Perylene-d12	14.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	53
2	1-Cyclohexene, 1,3,3-trimethyl-2...	206	C14H22O	1000197-08-4	47
3	1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	38
4	Anthracene, 9-[2,2-bis(hydroxyme...	280	C19H20O2	144000-85-1	35
5	Acetamide, N-[3-[[(2,5-dioxo-1-p...	303	C16H21N3O3	027550-64-7	35





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Acq On : 9 Aug 2017 00:27
Operator : SJ/JU
Sample : I4657-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-01-080717-A

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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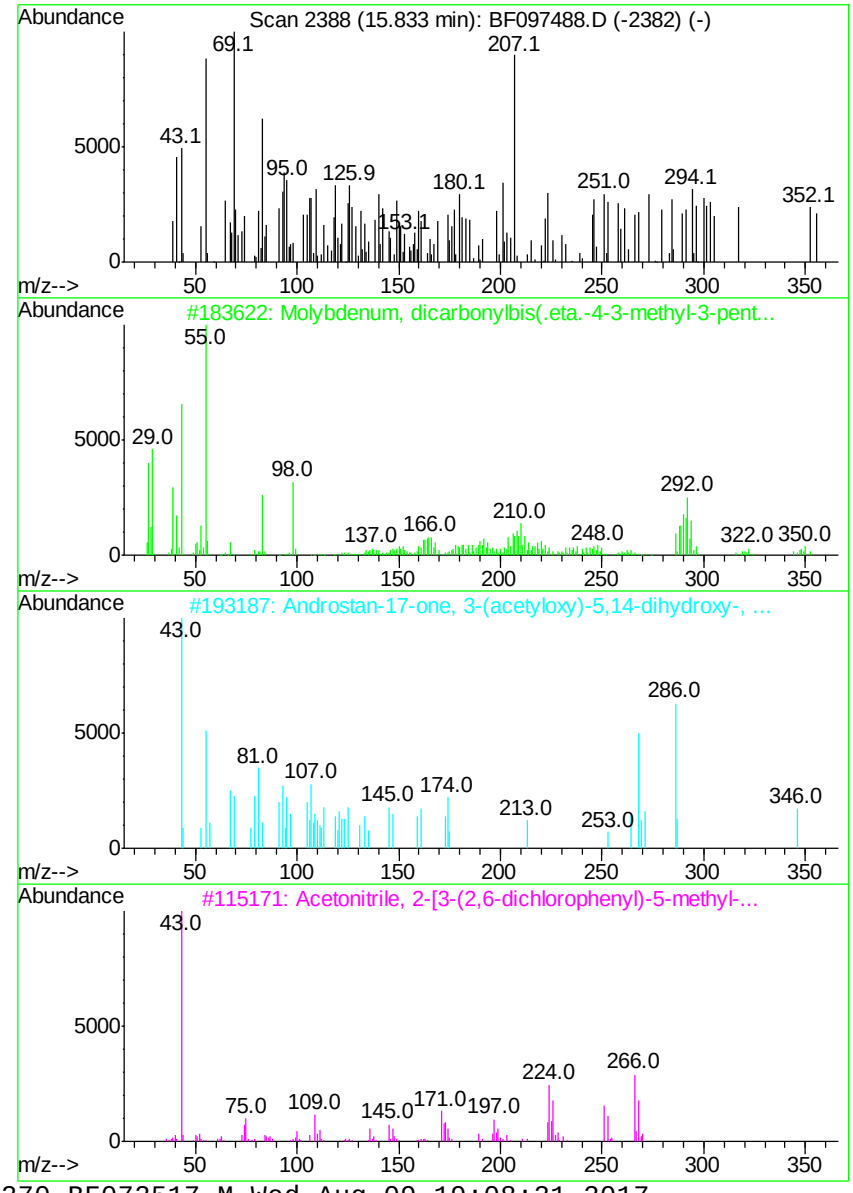
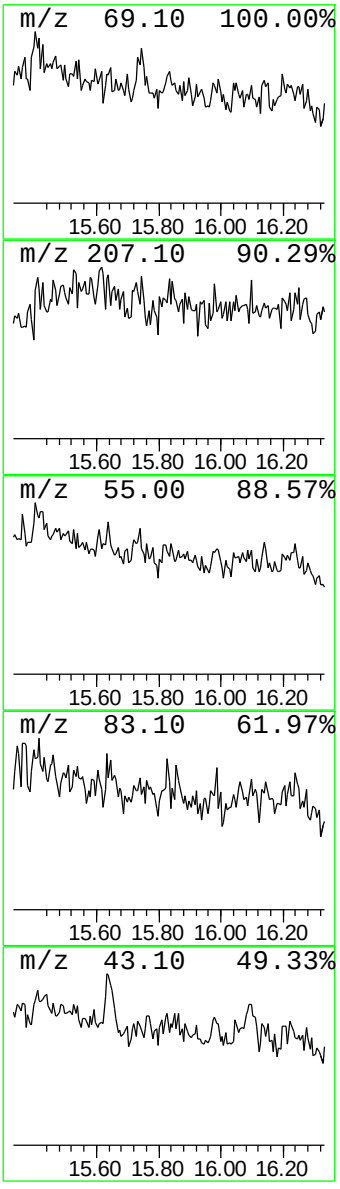
Peak Number 12 unknown15.83 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.83	4.04 ng	92505	Perylene-d12	14.87

Hit# of 3	Tentative ID	MW	MolForm	CAS#	Qual
1	Molybdenum, dicarbonylbis(.eta.-...	350	C14H20MoO4	1000162-96-5	9
2	Androstan-17-one, 3-(acetyloxy)-...	364	C21H32O5	041853-32-1	9
3	Acetonitrile, 2-[3-(2,6-dichloro...	266	C12H8Cl2N2O	1000264-41-5	2





Library Search Compound Report

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Data File : BF097488.D
Acq On : 9 Aug 2017 00:27
Operator : SJ/JU
Sample : I4657-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-01-080717-A

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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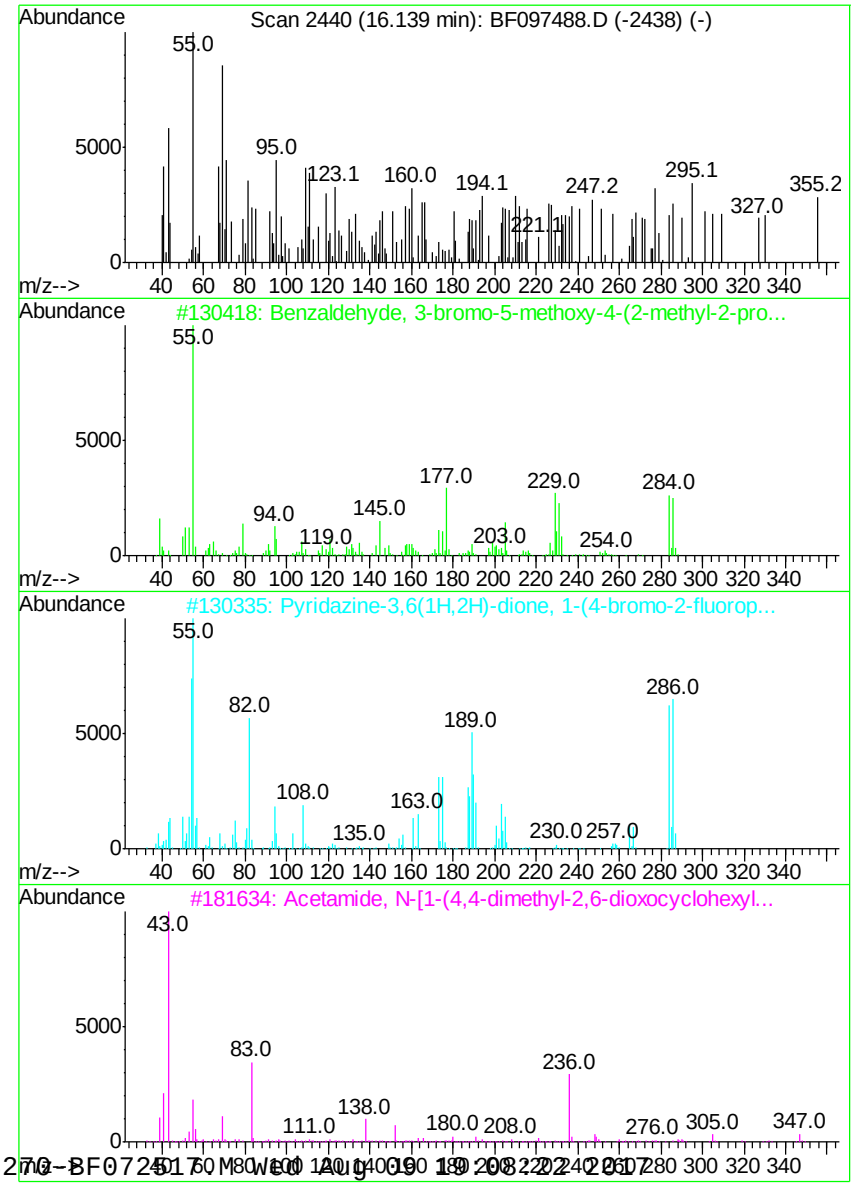
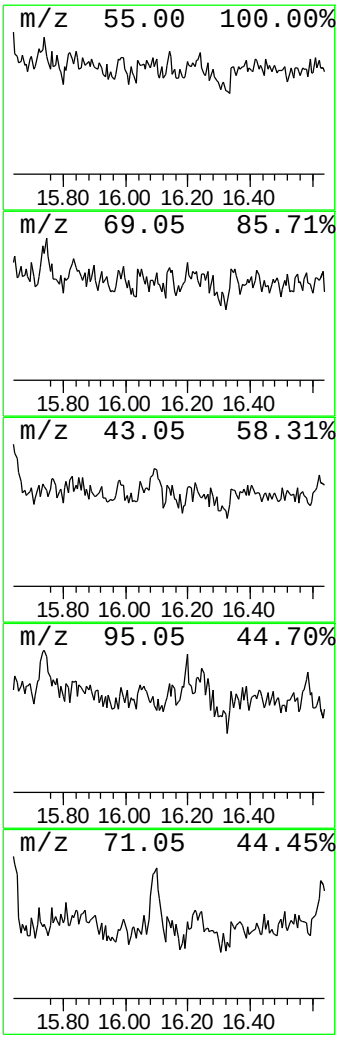
Peak Number 13 unknown16.14 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.14	2.36 ng	53997	Perylene-d12	14.87

Hit# of 4	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzaldehyde, 3-bromo-5-methoxy-...	284	C12H13BrO3	1000276-70-0	9
2	Pyridazine-3,6(1H,2H)-dione, 1-(...	284	C10H6BrFN2O2	1000272-67-6	9
3	Acetamide, N-[1-(4,4-dimethyl-2,...	347	C13H15F6NO3	1000362-54-7	4
4	Ethyl bis(2,4-dinitrophenyl) ace...	420	C16H12N4O10	005833-18-1	2





Library Search Compound Report

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Data File : BF097488.D
Acq On : 9 Aug 2017 00:27
Operator : SJ/JU
Sample : I4657-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-01-080717-A

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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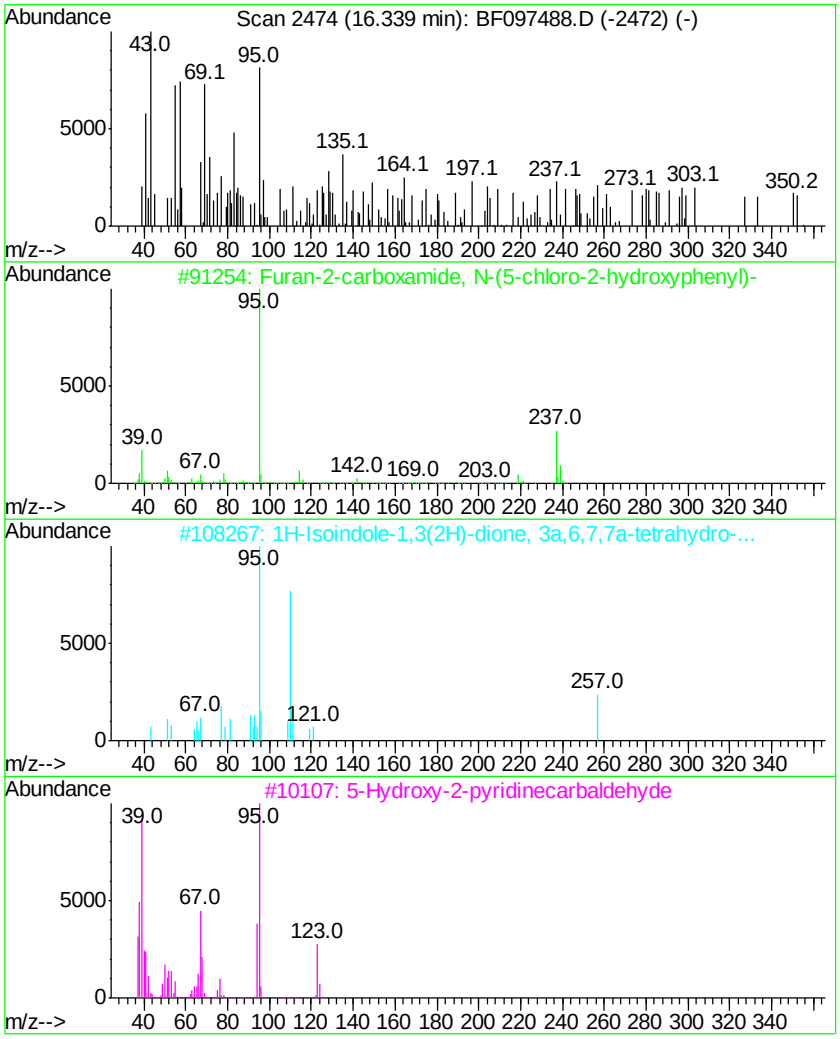
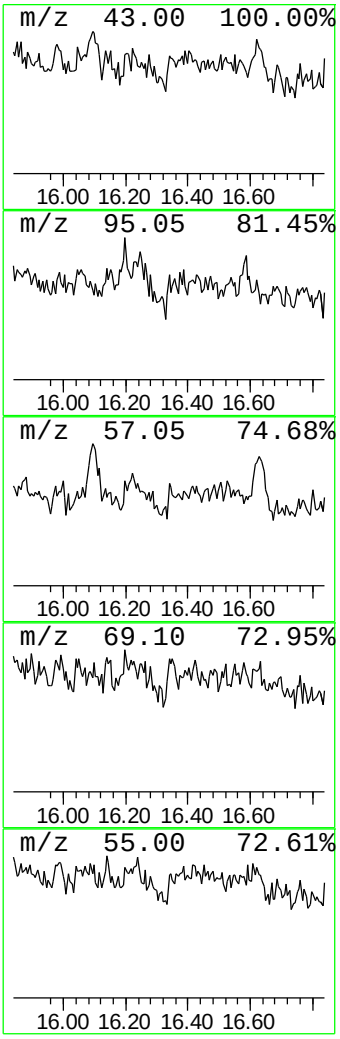
Peak Number 14 unknown16.34 Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.34	2.18 ng	49819	Perylene-d12	14.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Furan-2-carboxamide, N-(5-chloro...	237	C11H8ClNO3	075748-60-6	35
2	1H-Isoindole-1,3(2H)-dione, 3a,6...	257	C15H15NO3	054346-14-4	25
3	5-Hydroxy-2-pyridinecarbaldehyde	123	C6H5NO2	031191-08-9	25
4	4-(2-Methylcyclohex-1-enyl)-but-...	164	C11H16O	1000188-10-0	22
5	5-Octen-2-yn-4-ol	124	C8H12O	1000196-87-1	22





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Acq On : 9 Aug 2017 00:27
Operator : SJ/JU
Sample : I4657-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-01-080717-A

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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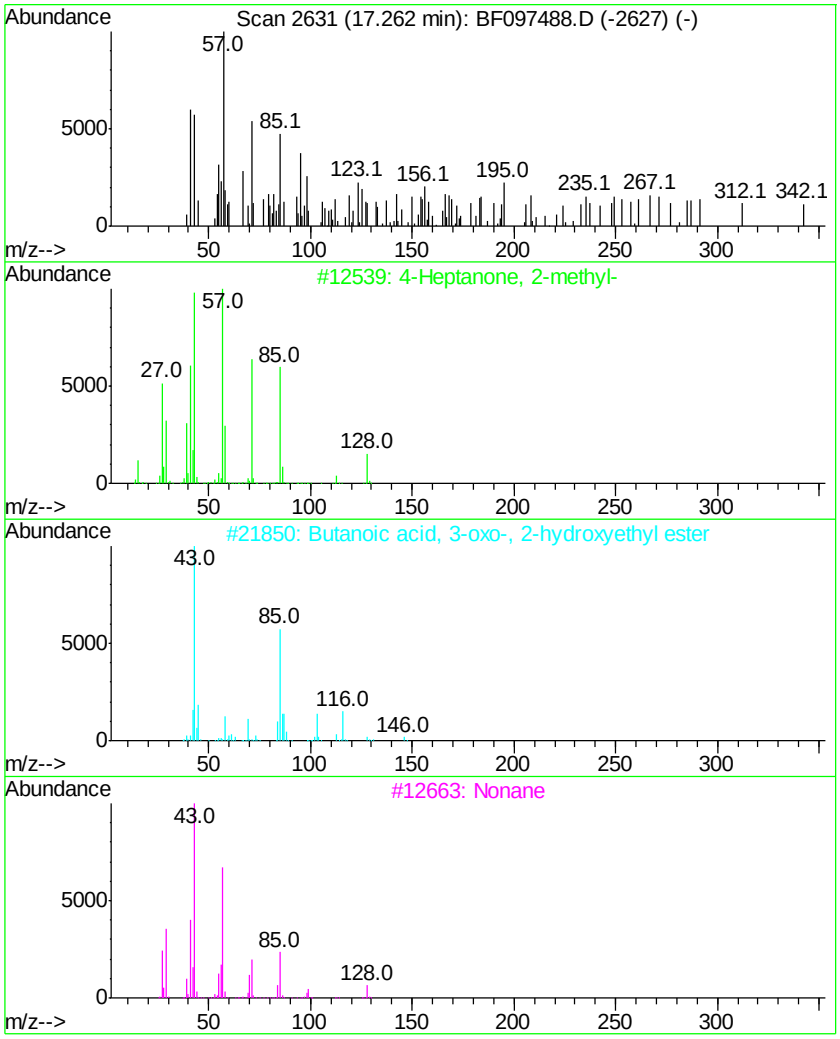
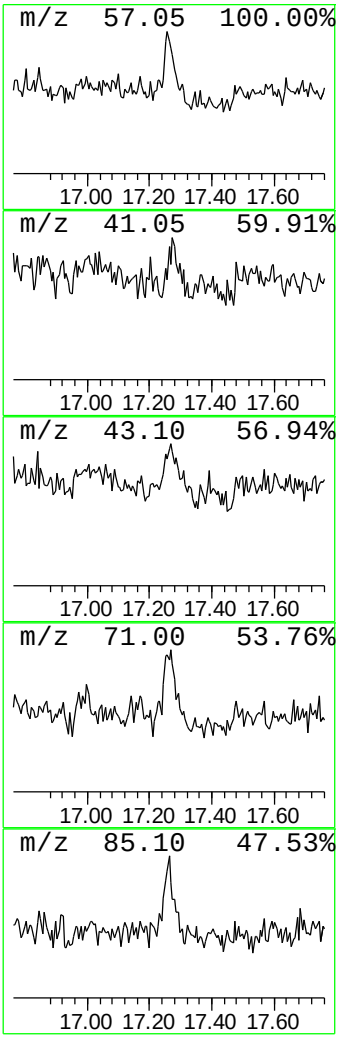
Peak Number 15 unknown17.26 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.26	2.31 ng	52885	Perylene-d12	14.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Heptanone, 2-methyl-	128	C8H16O	000626-33-5	11
2	Butanoic acid, 3-oxo-, 2-hydroxy...	146	C6H10O4	033736-01-5	10
3	Nonane	128	C9H20	000111-84-2	10
4	Hexane, 1,1'-oxybis-	186	C12H26O	000112-58-3	10
5	4,6-Dioxoheptanoic acid	158	C7H10O4	051568-18-4	10





Library Search Compound Report

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Data File : BF097488.D
Acq On : 9 Aug 2017 00:27
Operator : SJ/JU
Sample : I4657-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-01-080717-A

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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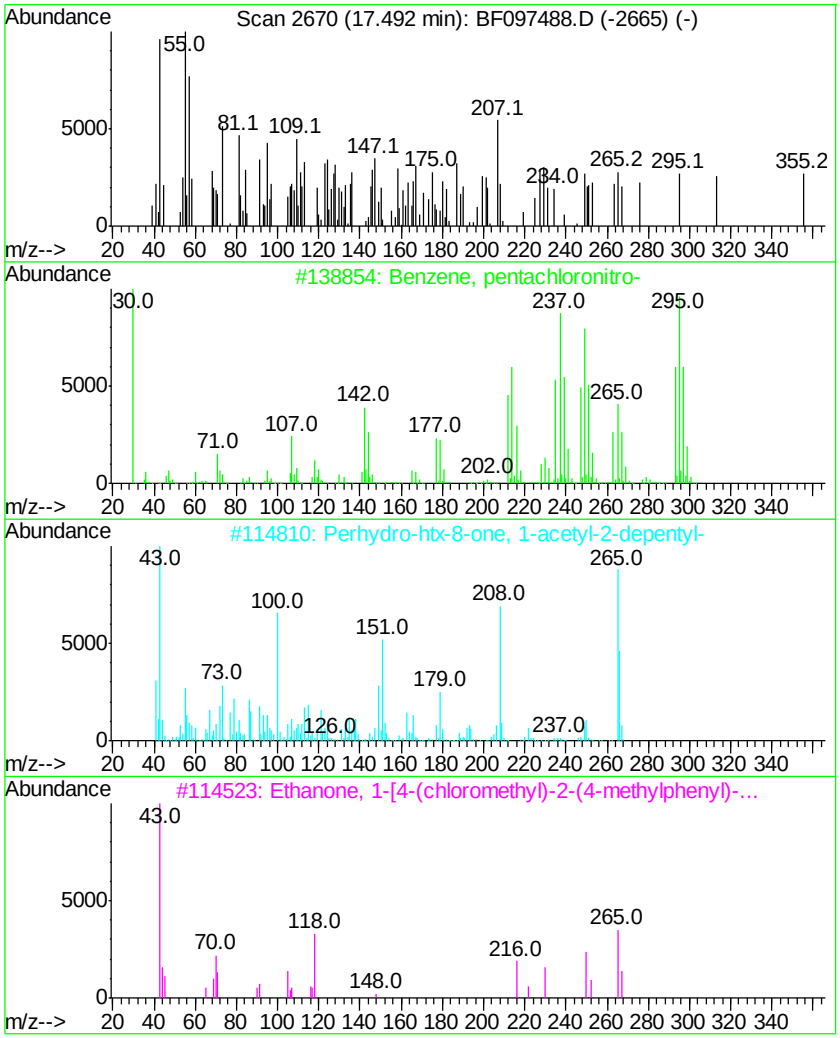
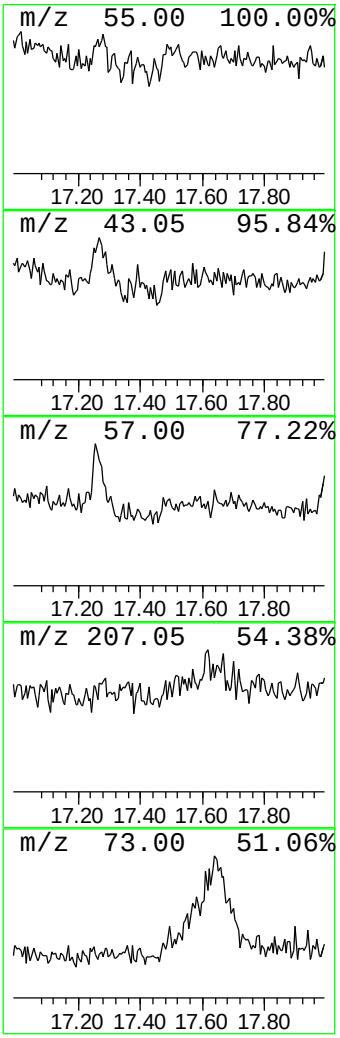
Peak Number 16 unknown17.49 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.49	2.31 ng	52768	Perylene-d12	14.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, pentachloronitro-	293	C6Cl5NO2	000082-68-8	14
2	Perhydro-htx-8-one, 1-acetyl-2-d...	265	C16H27NO2	082267-11-6	10
3	Ethanone, 1-[4-(chloromethyl)-2-...	265	C13H12ClNOS	041991-34-8	10
4	1-(5-Bromo-4-nitro-2-thienyl)eth...	249	C6H4BrNO3S	002160-55-6	9
5	2-Aminosuccinic acid, 2-benzyl-N...	363	C20H29NO5	079435-85-1	9





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Sample : I4657-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-01-080717-A

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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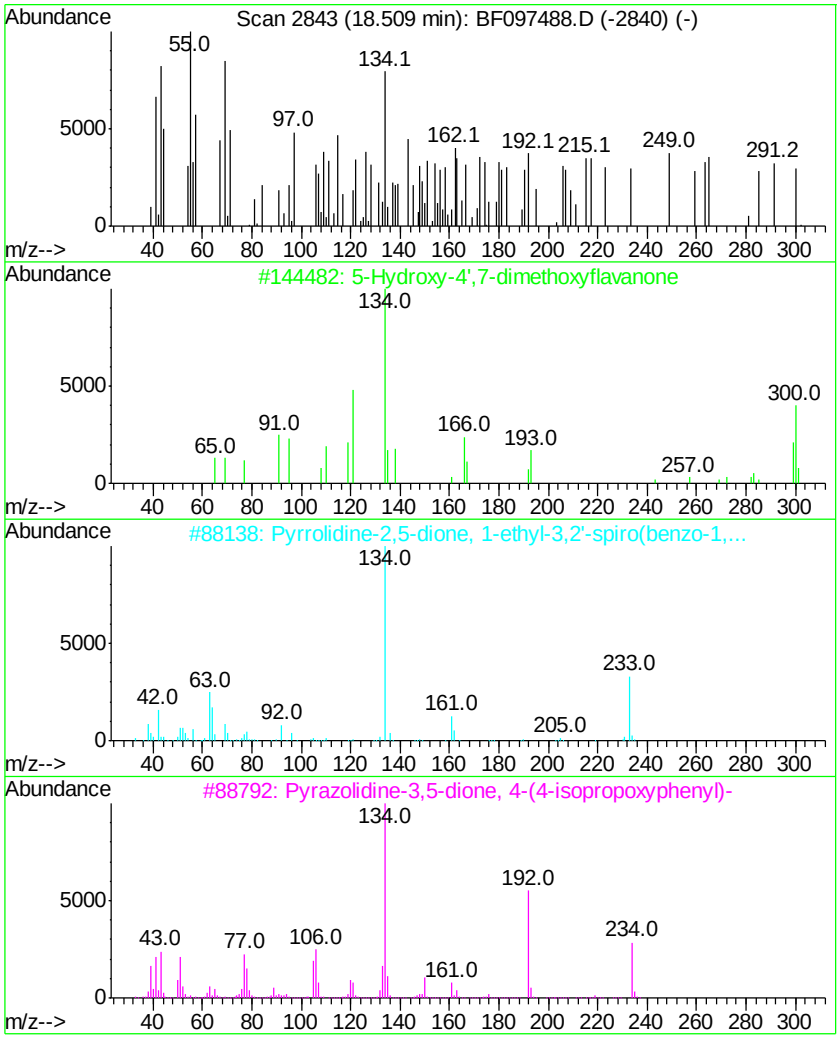
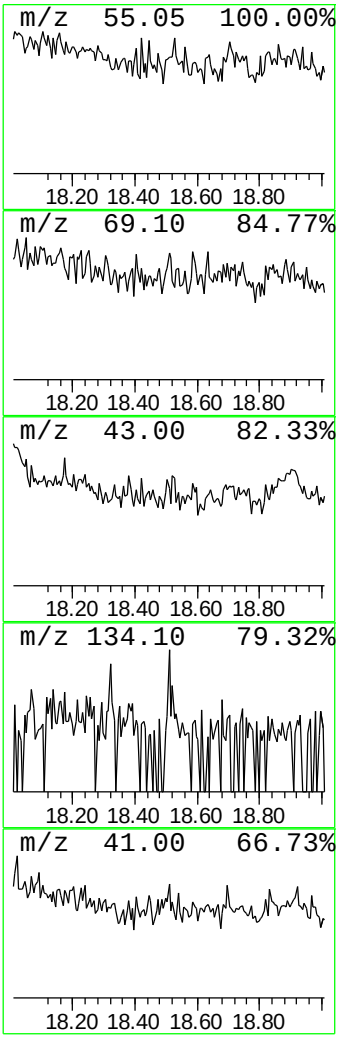
Peak Number 17 unknown18.51 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.51	2.26 ng	51672	Perylene-d12	14.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Hydroxy-4',7-dimethoxyflavanone	300	C17H16O5	069097-96-7	27
2	Pyrrolidine-2,5-dione, 1-ethyl-3...	233	C12H11NO4	109163-46-4	22
3	Pyrazolidine-3,5-dione, 4-(4-iso...	234	C12H14N2O3	1000259-14-4	22
4	Quinoxaline, 1,4-diacetyl-1,2,3,...	291	C14H17N3O4	1000350-39-3	18
5	Benzimidazole, 2-ethoxy-	162	C9H10N2O	022219-23-4	18





Tentatively Identified Compound (LSC) summary

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Data File : BF097488.D
Acq On : 9 Aug 2017 00:27
Operator : SJ/JU
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Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
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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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.53	4.2	ng	134399	1	6.40	642501	20.0
unknown6.18	6.18	46.4	ng	1490760	1	6.40	642501	20.0
4H-Cyclopenta[def...	11.52	2.1	ng	62496	4	10.90	605322	20.0
Squalene	14.37	4.7	ng	108263	6	14.87	457646	20.0
unknown14.44	14.44	4.5	ng	104059	6	14.87	457646	20.0
unknown14.63	14.63	4.5	ng	102490	6	14.87	457646	20.0
Benzo[e]pyrene	14.77	2.6	ng	59307	6	14.87	457646	20.0
unknown14.96	14.96	3.9	ng	88557	6	14.87	457646	20.0
unknown15.40	15.40	3.0	ng	68996	6	14.87	457646	20.0
.beta.-iso-Methyl...	15.74	4.0	ng	90412	6	14.87	457646	20.0
unknown15.83	15.83	4.0	ng	92505	6	14.87	457646	20.0
unknown16.14	16.14	2.4	ng	53997	6	14.87	457646	20.0
unknown16.34	16.34	2.2	ng	49819	6	14.87	457646	20.0
unknown17.26	17.26	2.3	ng	52885	6	14.87	457646	20.0
unknown17.49	17.49	2.3	ng	52768	6	14.87	457646	20.0
unknown18.51	18.51	2.3	ng	51672	6	14.87	457646	20.0