LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072817\
Data File : BF097153.D
Acq On : 28 Jul 2017 14:38
Operator : SJ/JU
Sample : I4397-06 2X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T-1C-14.5-15.0-072117

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	2.622	123	125	135	rBV	37622	107907	7.62%	0.698%
2	4.616	461	464	473	rBV	93642	130790	9.23%	0.846%
3	5.081	539	543	565	rBV	1224156	1381984	97.54%	8.935%
4	6.145	721	724	739	rBV	1490385	1416822	100.00%	9.160%
5	6.257	739	743	755	rVB	1536378	1356966	95.78%	8.773%
6	6.487	778	782	791	rBV	803246	684222	48.29%	4.423%
7	6.639	805	808	817	rBV	1110107	999681	70.56%	6.463%
8	7.051	874	878	893	rBV	945140	819481	57.84%	5.298%
9	7.186	899	901	909	rVB3	17029	22260	1.57%	0.144%
10	7.698	985	988	992	rBV	31430	30339	2.14%	0.196%
11	7.769	996	1000	1005	rBV	1105097	905713	63.93%	5.855%
12	8.216	1073	1076	1083	rVB3	19423	22072	1.56%	0.143%
13	8.810	1175	1177	1179	rBV	22619	17820	1.26%	0.115%
14	8.845	1179	1183	1187	rBV	1518344	1260214	88.95%	8.147%
15	8.945	1197	1200	1206	rVB	24860	26157	1.85%	0.169%
16	9.245	1248	1251	1253	rBV	218712	163658	11.55%	1.058%
17	9.263	1253	1254	1257	rVB	40392	26519	1.87%	0.171%
18	9.475	1286	1290	1292	rBV	37117	33699	2.38%	0.218%
19	9.516	1293	1297	1300	rVV	915544	821754	58.00%	5.313%
20	9.545	1300	1302	1307	rVB6	18860	18746	1.32%	0.121%
21	9.704	1321	1329	1331	rBV6	12639	27150	1.92%	0.176%
22	9.792	1341	1344	1347	rBV	24864	20456	1.44%	0.132%
23	9.945	1367	1370	1372	rBV	42853	38979	2.75%	0.252%
24	9.969	1372	1374	1377	rVB	63382	45875	3.24%	0.297%
25	10.186	1404	1411	1415	rBV	69393	96985	6.85%	0.627%
26	10.298	1427	1430	1436	rBV	685705	616028	43.48%	3.983%
27	10.451	1451	1456	1463	rBV	120631	178969	12.63%	1.157%
28	10.633	1484	1487	1490	rBV3	26277	30805	2.17%	0.199%
29	10.886	1527	1530	1532	rBV	66464	55158	3.89%	0.357%
30	10.916	1532	1535	1539	rVB	52712	51318	3.62%	0.332%
31	10.986	1543	1547	1550	rBV	722150	614226	43.35%	3.971%
32	11.010	1550	1551	1555	rVB	81676	50806	3.59%	0.328%
33	11.063	1557	1560	1565	rVB2	21422	18774	1.33%	0.121%
34	11.310	1599	1602	1607	rBV	48989	45240	3.19%	0.292%

LSC Area Percent Report

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Operator : SJ/JU
Sample : I4397-06 2X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T-1C-14.5-15.0-072117

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	11.486	1624	1632	1635	rBV9	17332	32833	2.32%	0.212%
36	11.539	1640	1641	1644	rBV2	19571	16194	1.14%	0.105%
37	11.598	1649	1651	1653	rBV2	15170	14779	1.04%	0.096%
38	11.716	1668	1671	1678	rVB	45271	45161	3.19%	0.292%
39	11.810	1685	1687	1692	rVB4	14237	15424	1.09%	0.100%
40	12.098	1733	1736	1739	rBV	38450	32980	2.33%	0.213%
41	12.192	1749	1752	1758	rVB	137034	120729	8.52%	0.781%
42	12.333	1772	1776	1779	rVB6	10457	16123	1.14%	0.104%
43	12.416	1786	1790	1793	rBV	126572	113442	8.01%	0.733%
44	12.468	1797	1799	1805	rVV2	39761	45934	3.24%	0.297%
45	12.568	1812	1816	1822	rVB	945948	835221	58.95%	5.400%
46	12.821	1856	1859	1862	rVB2	26670	29635	2.09%	0.192%
47	12.851	1862	1864	1868	rVB3	19350	23562	1.66%	0.152%
48	12.951	1876	1881	1882	rBV3	16364	22215	1.57%	0.144%
49	12.974	1882	1885	1889	rVV5	16600	21751	1.54%	0.141%
50	13.168	1915	1918	1920	rVB	26814	24544	1.73%	0.159%
51	13.257	1931	1933	1935	rVB	22823	19668	1.39%	0.127%
52	13.363	1947	1951	1952	rBV3	12890	19247	1.36%	0.124%
53	13.492	1969	1973	1978	rVB2	57444	77331	5.46%	0.500%
54	13.610	1989	1993	1996	rBV	728223	729033	51.46%	4.713%
55	13.633	1996	1997	2001	rVB	56661	43954	3.10%	0.284%
56	13.721	2010	2012	2013	rBV2	21408	19209	1.36%	0.124%
57	13.810	2025	2027	2029	rVB	28279	23103	1.63%	0.149%
58	13.957	2049	2052	2053	rBV3	20043	21313	1.50%	0.138%
59	14.115	2074	2079	2084	rBV6	56818	142276	10.04%	0.920%
60	14.762	2186	2189	2191	rBV3	68903	86144	6.08%	0.557%
61	14.962	2219	2223	2229	rBV	456839	522431	36.87%	3.378%
62	16.609	2501	2503	2506	rBV3	43912	48078	3.39%	0.311%
63	16.792	2533	2534	2535	rBV	45486	31784	2.24%	0.205%
64	17.515	2654	2657	2659	rBV3	40908	55135	3.89%	0.356%
65	18.009	2739	2741	2743	rBV3	34715	43704	3.08%	0.283%
66	18.621	2843	2845	2846	rBV2	37081	37438	2.64%	0.242%

Sum of corrected areas: 15467948

LSC Report - Integrated Chromatogram

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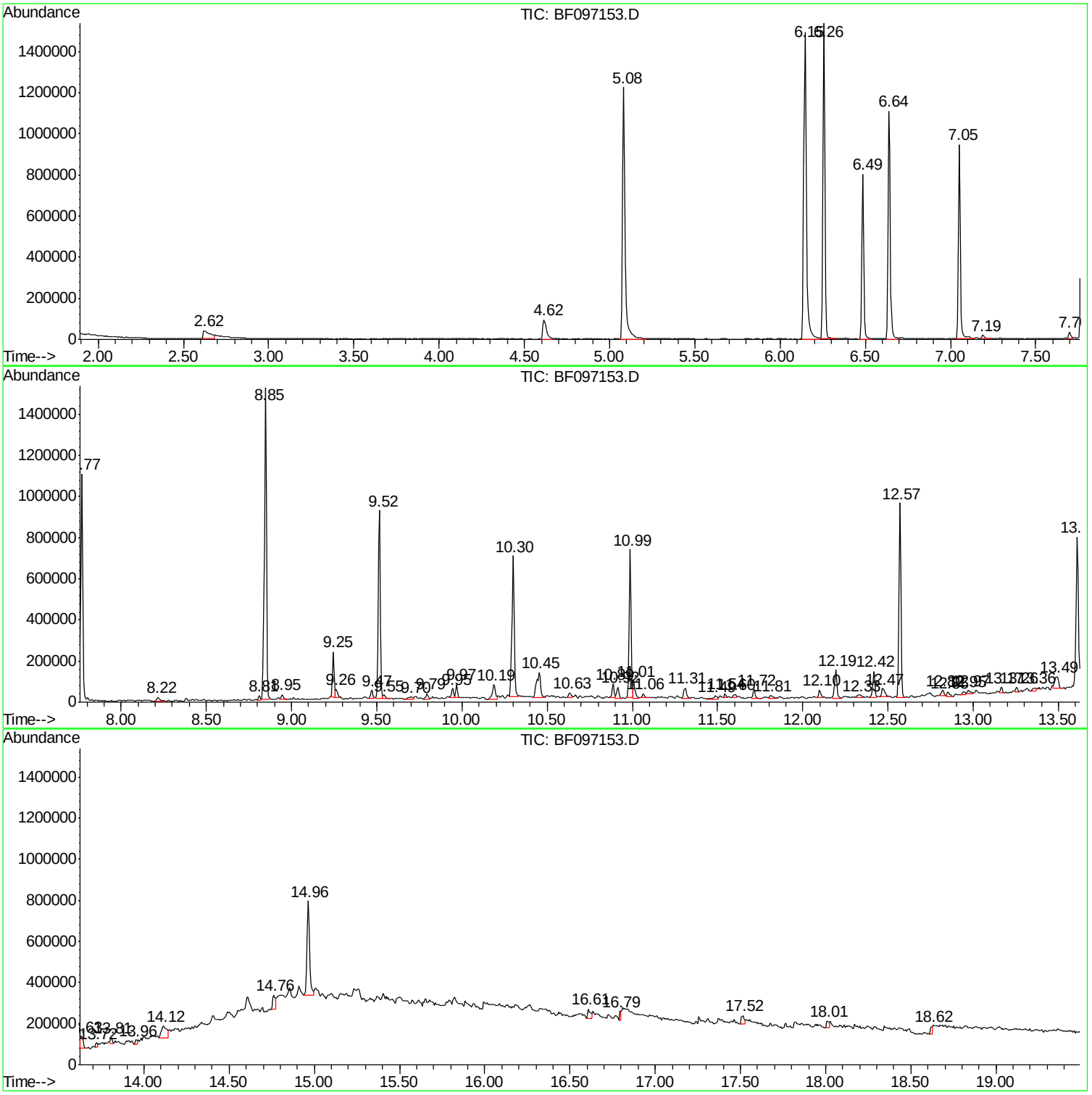
Data File : BF097153.D
Acq On : 28 Jul 2017 14:38
Operator : SJ/JU
Sample : I4397-06 2X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
T-1C-14.5-15.0-072117

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

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Data File : BF097153.D
Acq On : 28 Jul 2017 14:38
Operator : SJ/JU
Sample : I4397-06 2X
Misc :
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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

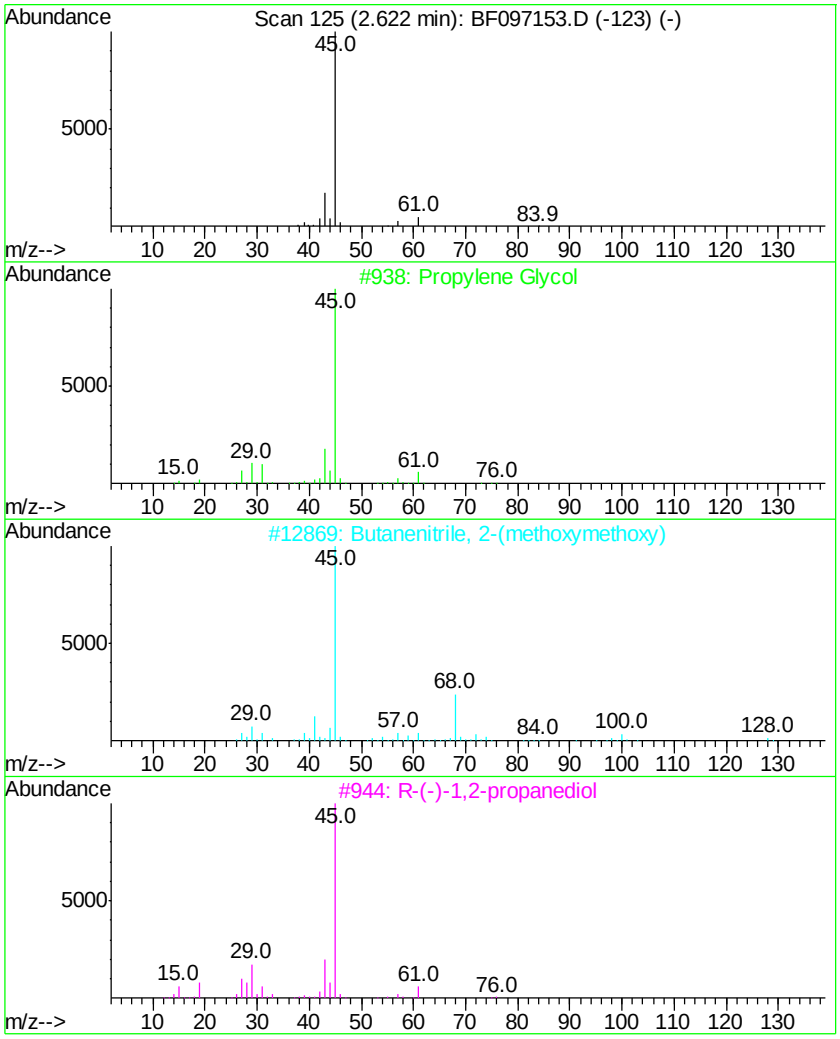
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

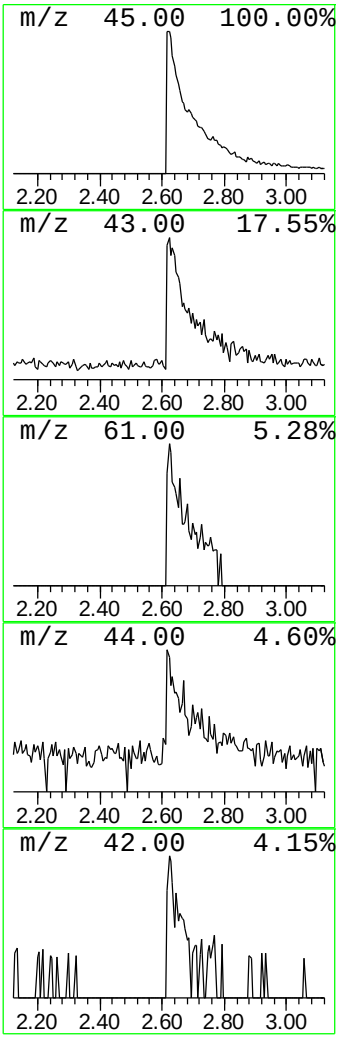
****

Peak Number 1 unknown2.62 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.62	3.15 ng	107907	1,4-Dichlorobenzene-d4	6.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	9
2	Butanenitrile, 2-(methoxymethoxy)	129	C6H11NO2	1000196-86-5	9
3	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	9
4	Isopropyl Alcohol	60	C3H8O	000067-63-0	9
5	Formamide	45	CH3NO	000075-12-7	7





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072817\
Data File : BF097153.D
Acq On : 28 Jul 2017 14:38
Operator : SJ/JU
Sample : I4397-06 2X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T-1C-14.5-15.0-072117

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

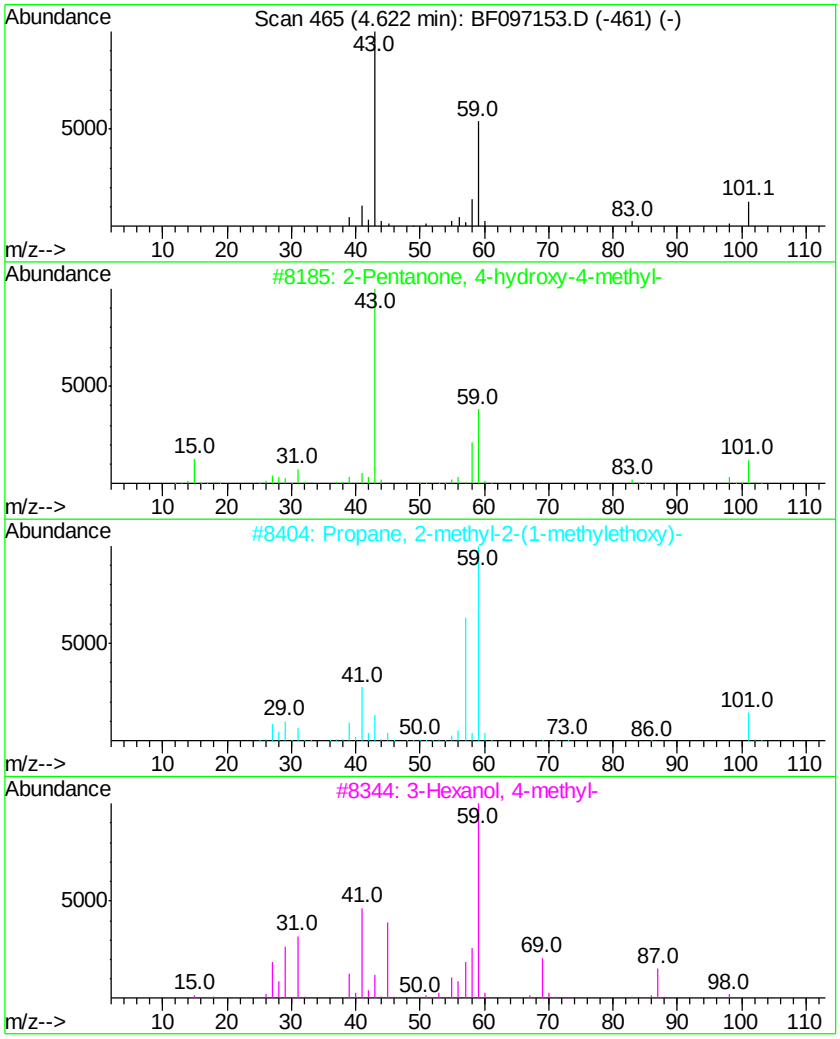
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

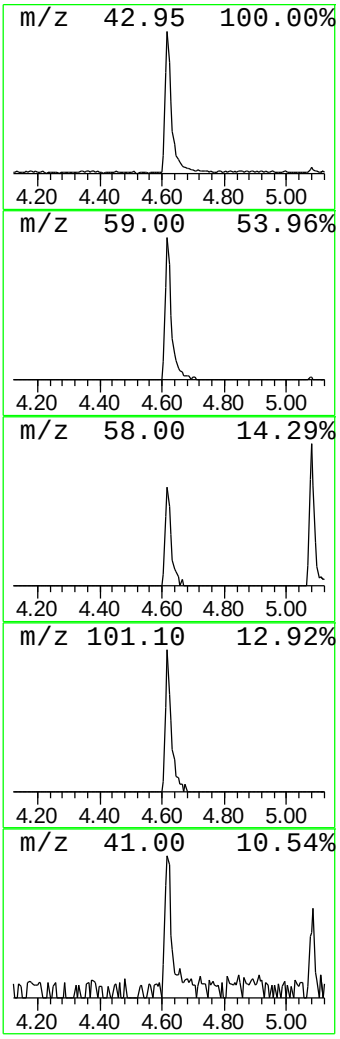
****

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.62	3.82 ng	130790	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	64
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27





Data Path : Z:\HPCHEM1\BNA F\DATA\BF072817\
Data File : BF097153.D
Acq On : 28 Jul 2017 14:38
Operator : SJ/JU
Sample : I4397-06 2X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T-1C-14.5-15.0-072117

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

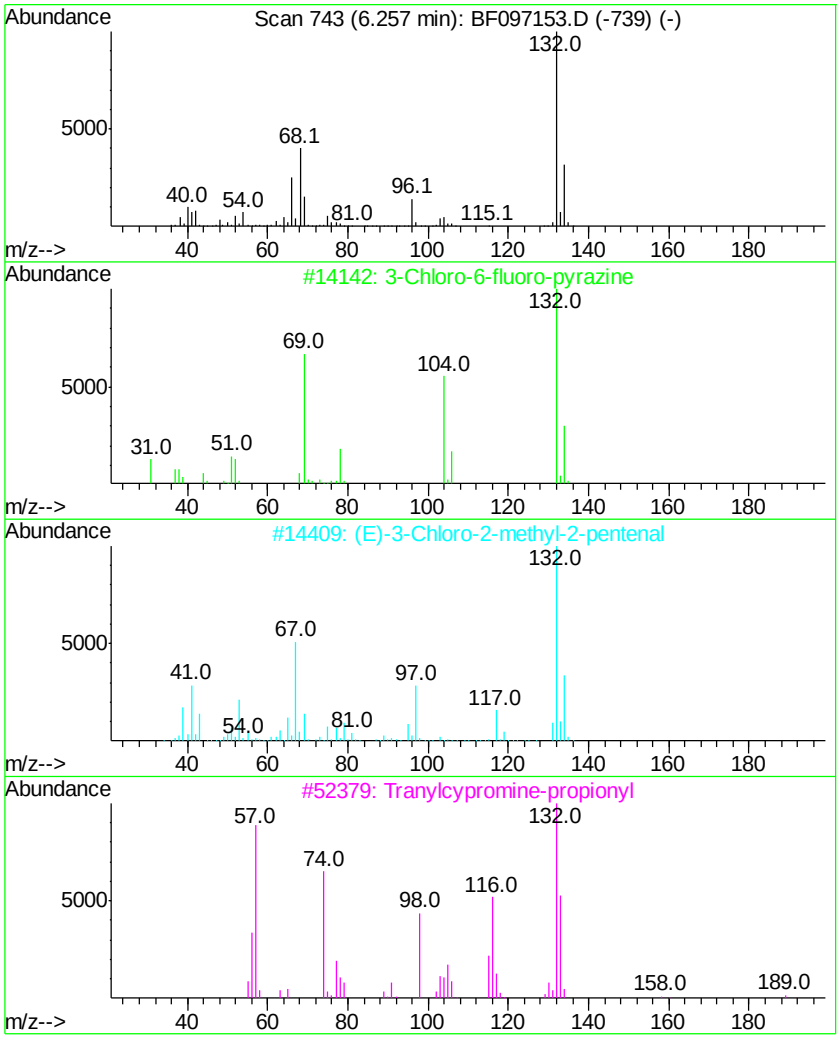
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

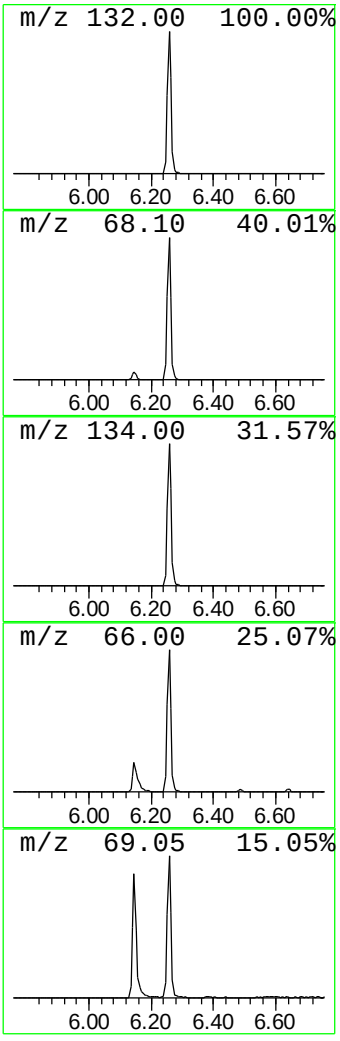
****

Peak Number 3 unknown6.26 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.26	39.66 ng	1356970	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	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





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Misc :
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Instrument : BNA_F
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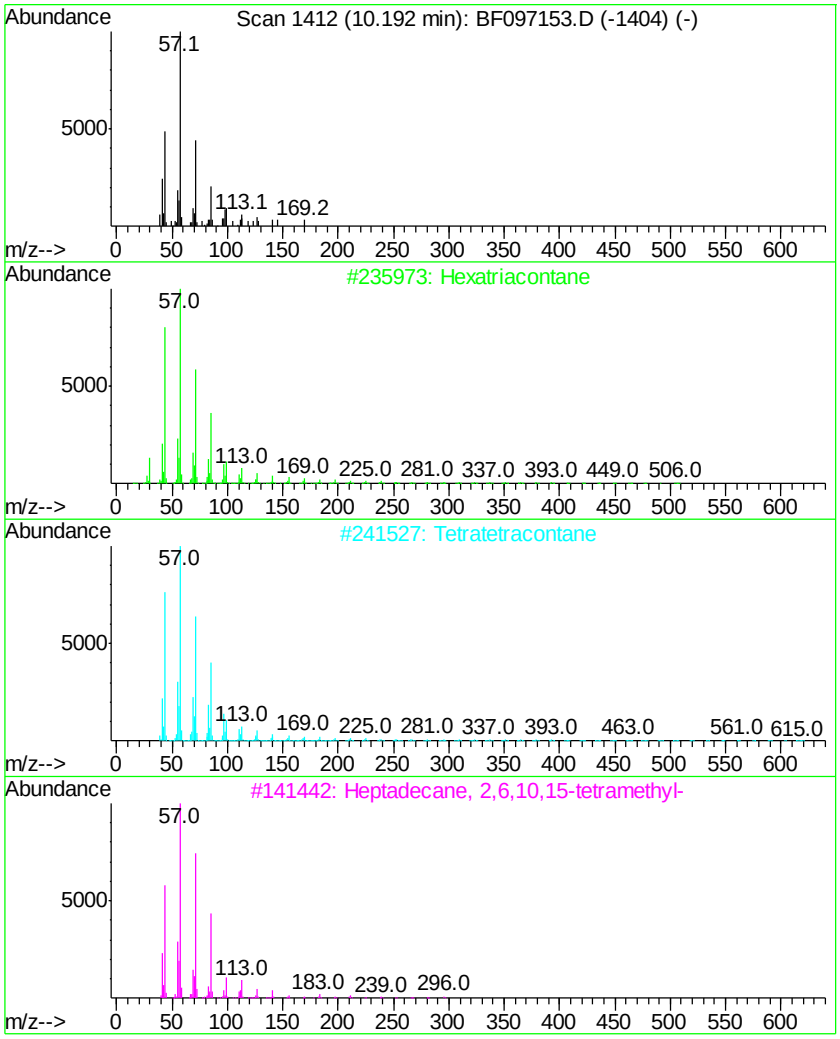
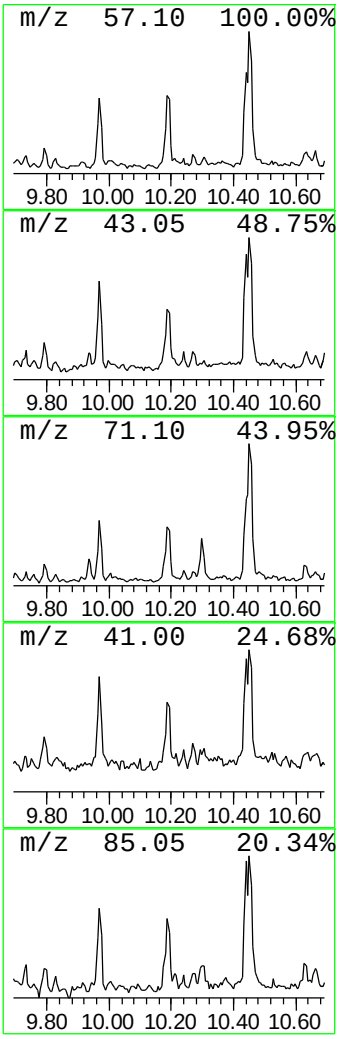
****

Peak Number 5 Hexatriacontane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.19	2.36 ng	96985	Acenaphthene-d10	9.52

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexatriacontane	507	C36H74	000630-06-8	80
2	Tetratetracontane	619	C44H90	007098-22-8	80
3	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	80
4	Octacosane	394	C28H58	000630-02-4	72
5	Heneicosane	296	C21H44	000629-94-7	72





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Sample : I4397-06 2X
Misc :
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Instrument : BNA_F
ClientSampleId : T-1C-14.5-15.0-072117

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

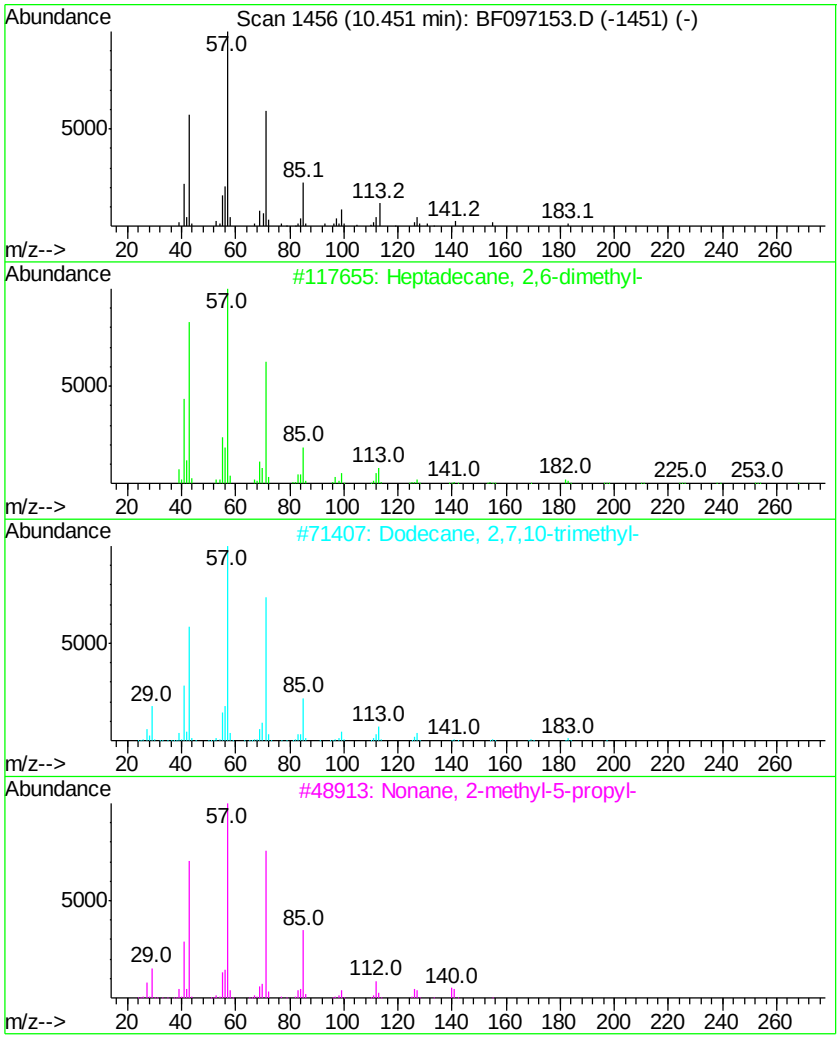
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

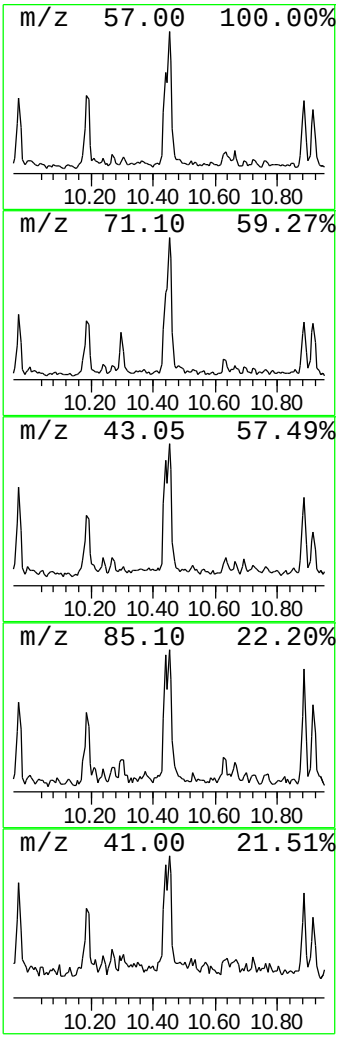
****

Peak Number 6 Heptadecane, 2,6-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.45	5.83 ng	178969	Phenanthrene-d10	10.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 2,6-dimethyl-	268	C19H40	054105-67-8	83
2	Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	80
3	Nonane, 2-methyl-5-propyl-	184	C13H28	031081-17-1	64
4	Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	59
5	Sulfurous acid, 2-ethylhexyl non...	320	C17H36O3S	1000309-19-2	58





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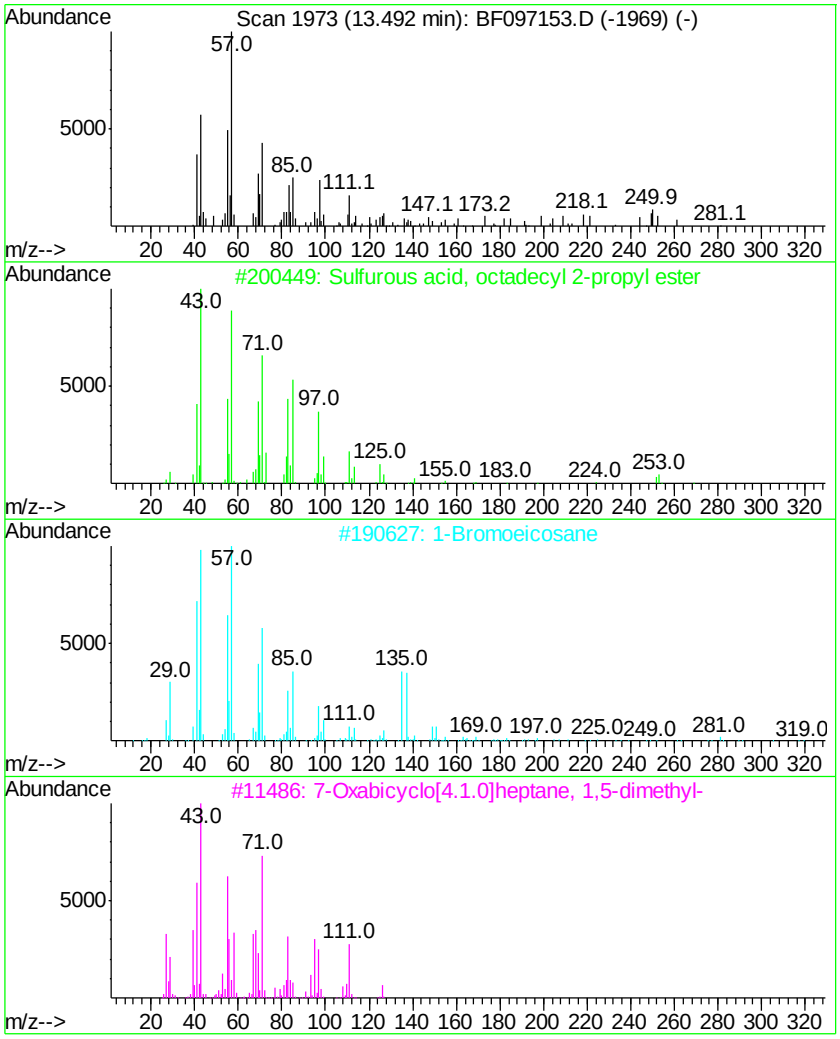
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

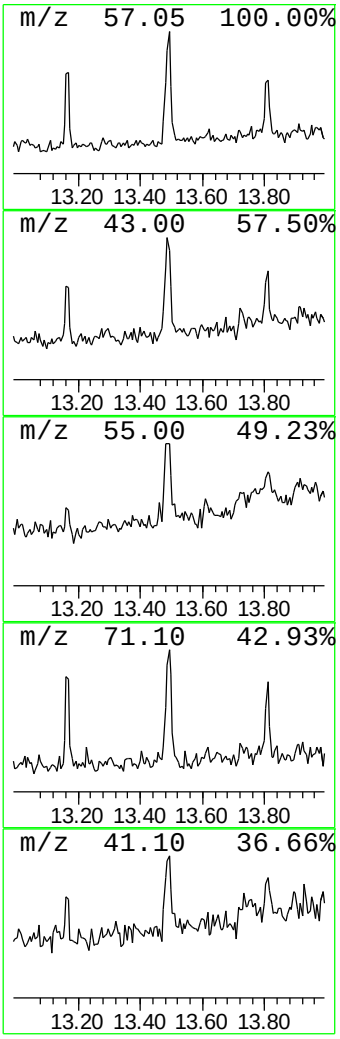
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Sulfurous acid, octadecyl 2... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.49	2.12 ng	77331	Chrysene-d12	13.61

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	64
2	1-Bromoeicosane	360	C20H41Br	004276-49-7	47
3	7-Oxabicyclo[4.1.0]heptane, 1,5-...	126	C8H14O	162239-52-3	43
4	Dodecane, 1-bromo-	248	C12H25Br	000143-15-7	43
5	Tetratetracontane	619	C44H90	007098-22-8	43





Data Path : Z:\HPCHEM1\BNA F\DATA\BF072817\
Data File : BF097153.D
Acq On : 28 Jul 2017 14:38
Operator : SJ/JU
Sample : I4397-06 2X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T-1C-14.5-15.0-072117

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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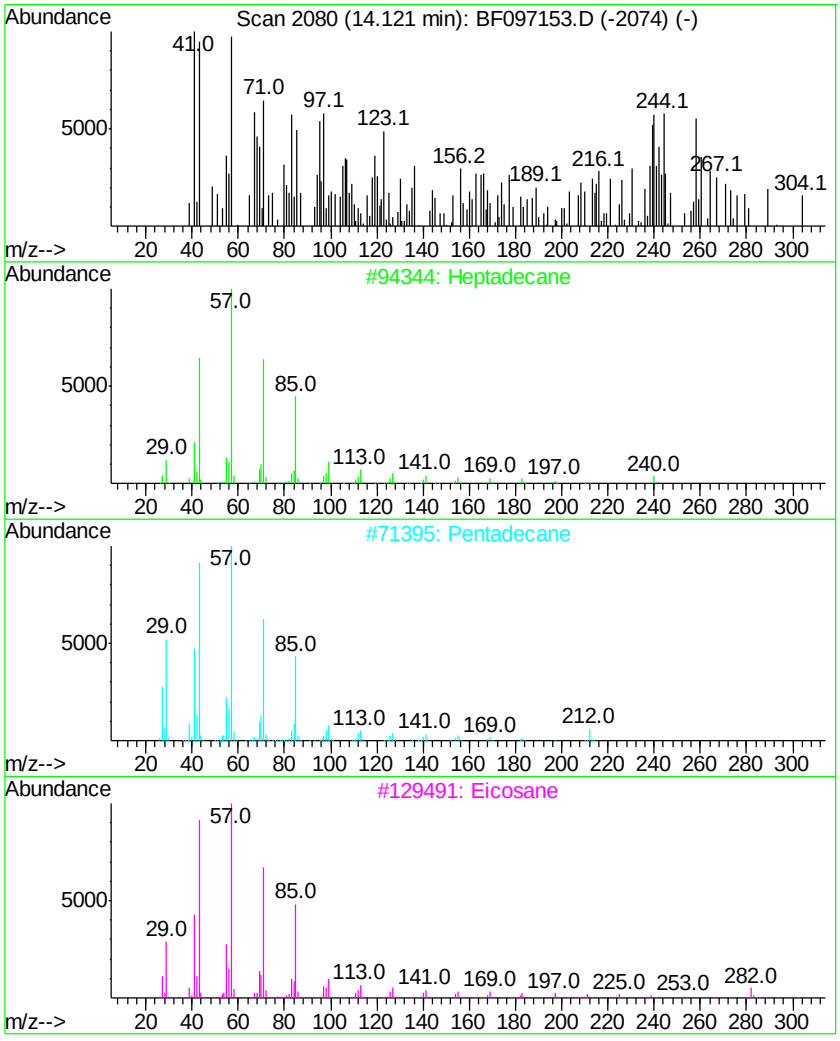
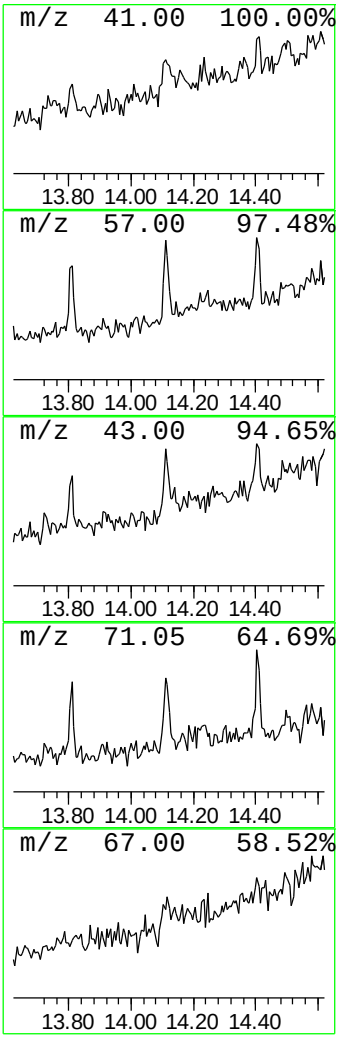
Peak Number 8 unknown14.12 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.12	3.90 ng	142276	Chrysene-d12	13.61

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	38
2	Pentadecane	212	C15H32	000629-62-9	25
3	Eicosane	282	C20H42	000112-95-8	25
4	Hexadecane	226	C16H34	000544-76-3	15
5	Tridecane	184	C13H28	000629-50-5	15





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072817\
Data File : BF097153.D
Acq On : 28 Jul 2017 14:38
Operator : SJ/JU
Sample : I4397-06 2X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T-1C-14.5-15.0-072117

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

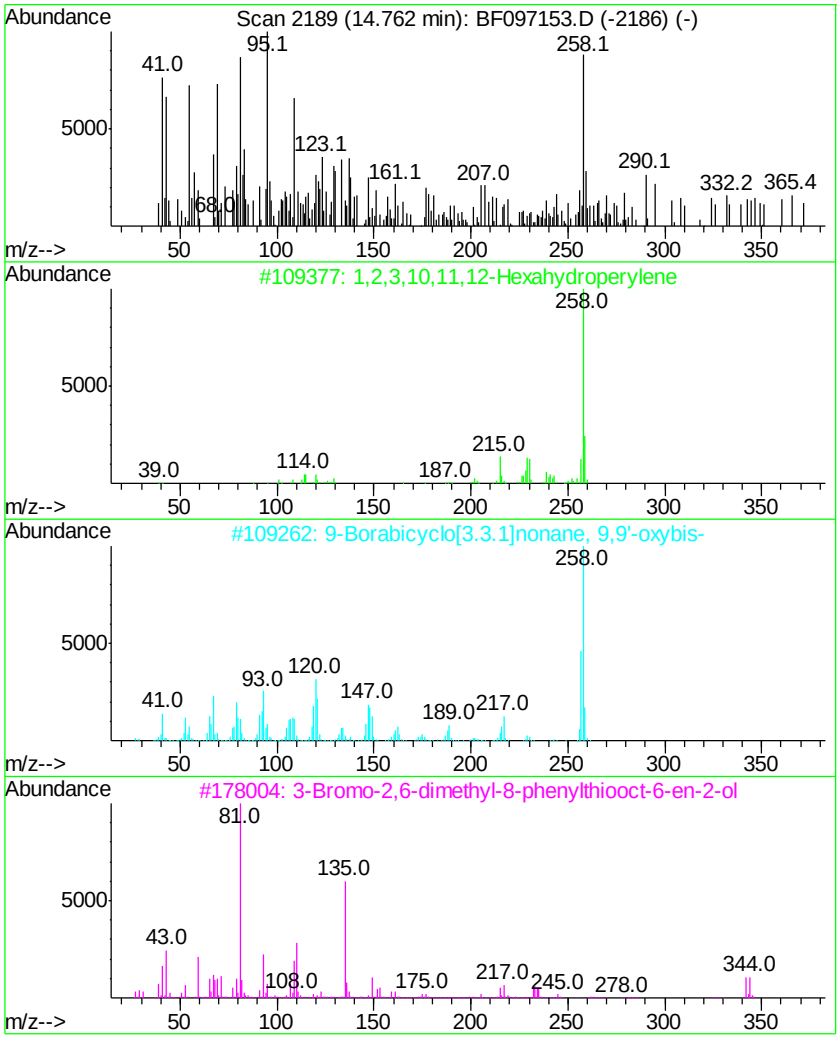
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

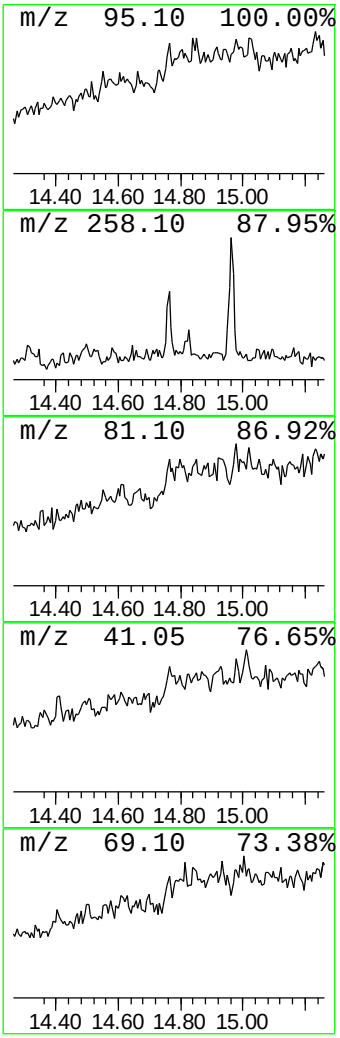
****

Peak Number 9 unknown14.76 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.76	3.30 ng	86144	Perylene-d12	14.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2,3,10,11,12-Hexahydroperylene	258	C20H18	007350-92-7	27
2	9-Borabicyclo[3.3.1]nonane, 9,9'...	258	C16H28B2O	074744-62-0	25
3	3-Bromo-2,6-dimethyl-8-phenylthi...	342	C16H23BrOS	113219-35-5	15
4	Ferrocene, (trimethylsilyl)-	258	C13H18FeSi	012215-68-8	15
5	Cyclohexanone, 2-(1-mercapto-1-m...	186	C10H18OS	033281-91-3	14





Data Path : Z:\HPCHEM1\BNA F\DATA\BF072817\
Data File : BF097153.D
Acq On : 28 Jul 2017 14:38
Operator : SJ/JU
Sample : I4397-06 2X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T-1C-14.5-15.0-072117

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

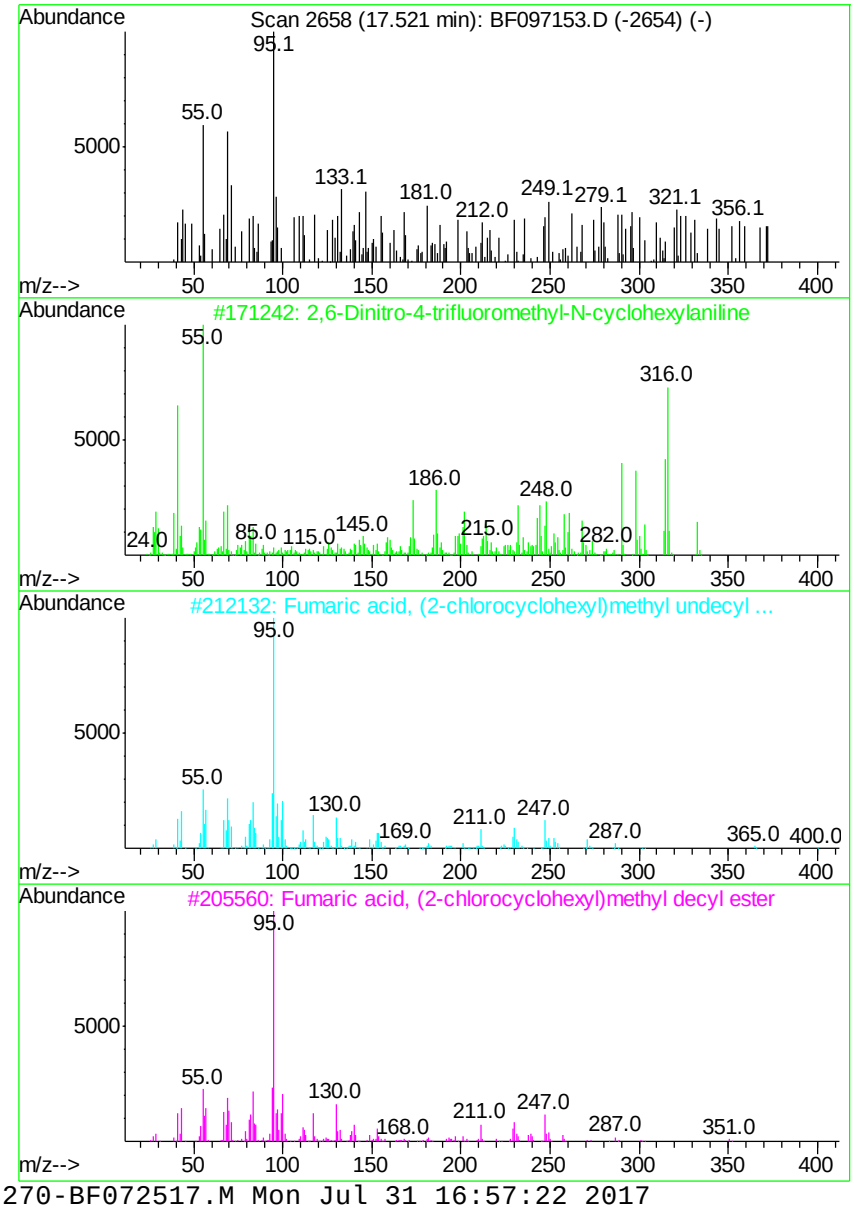
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

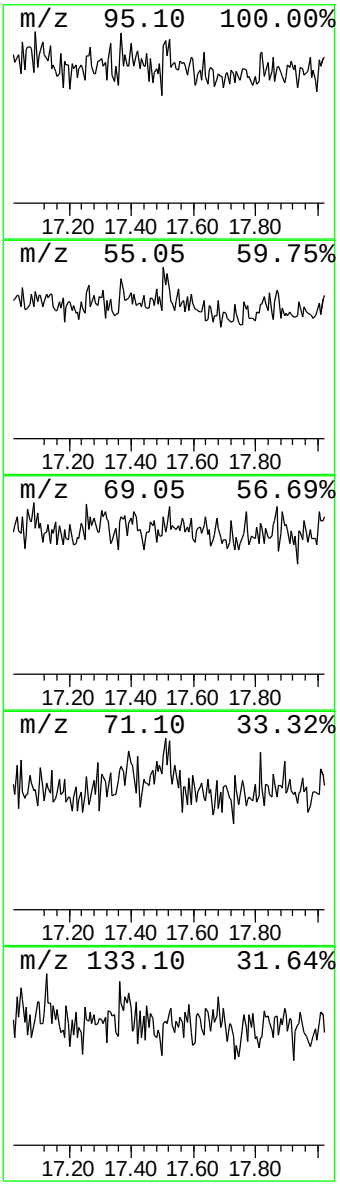
****

Peak Number 10 unknown17.52 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.52	2.11 ng	55135	Perylene-d12	14.96

Hit# of 3	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6-Dinitro-4-trifluoromethyl-N-...	333	C13H14F3N3O4	073015-58-4	9
2	Fumaric acid, (2-chlorocyclohexy...	400	C22H37ClO4	1000345-07-5	7
3	Fumaric acid, (2-chlorocyclohexy...	386	C21H35ClO4	1000345-07-4	1





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072817\
Data File : BF097153.D
Acq On : 28 Jul 2017 14:38
Operator : SJ/JU
Sample : I4397-06 2X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T-1C-14.5-15.0-072117

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
unknown2.62	2.62	3.1	ng	107907	1	6.49	684222	20.0
2-Pentanone, 4-hy...	4.62	3.8	ng	130790	1	6.49	684222	20.0
unknown6.26	6.26	39.7	ng	1356970	1	6.49	684222	20.0
Hexatriacontane	10.19	2.4	ng	96985	3	9.52	821754	20.0
Heptadecane, 2,6-...	10.45	5.8	ng	178969	4	10.99	614226	20.0
Sulfurous acid, o...	13.49	2.1	ng	77331	5	13.61	729033	20.0
unknown14.12	14.12	3.9	ng	142276	5	13.61	729033	20.0
unknown14.76	14.76	3.3	ng	86144	6	14.96	522431	20.0
unknown17.52	17.52	2.1	ng	55135	6	14.96	522431	20.0