LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072817\
Data File : BF097147.D
Acq On : 28 Jul 2017 11:52
Operator : SJ/JU
Sample : I4397-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T-1A-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	2.663	129	132	156	rBV	173699	372311	12.70%	1.407%
2	3.228	221	228	235	rVB2	21163	41652	1.42%	0.157%
3	4.640	464	468	480	rBV	177094	279642	9.54%	1.057%
4	5.093	540	545	566	rBV	2470761	2719111	92.78%	10.277%
5	6.151	720	725	739	rBV	2515032	2930621	100.00%	11.076%
6	6.263	739	744	747	rBV	2646996	2569097	87.66%	9.710%
7	6.487	778	782	793	rBV	779513	671269	22.91%	2.537%
8	6.645	804	809	812	rBV	1960442	1948242	66.48%	7.363%
9	7.057	874	879	882	rBV	1745535	1682757	57.42%	6.360%
10	7.192	898	902	906	rBV	34735	37728	1.29%	0.143%
11	7.692	984	987	996	rBV	49662	55717	1.90%	0.211%
12	7.769	996	1000	1004	rBV	1069704	918372	31.34%	3.471%
13	8.851	1178	1184	1187	rBV	2584657	2530183	86.34%	9.563%
14	9.245	1247	1251	1254	rBV	563572	436119	14.88%	1.648%
15	9.516	1292	1297	1300	rBV	1031582	907821	30.98%	3.431%
16	9.969	1371	1374	1377	rVB	51838	38430	1.31%	0.145%
17	10.186	1406	1411	1414	rBV2	20239	29715	1.01%	0.112%
18	10.304	1427	1431	1434	rBV	1443927	1422002	48.52%	5.374%
19	10.439	1450	1454	1460	rBV	72185	78319	2.67%	0.296%
20	10.886	1527	1530	1532	rVB	61331	48447	1.65%	0.183%
21	10.986	1543	1547	1549	rBV	880462	772275	26.35%	2.919%
22	11.010	1549	1551	1555	rVB	359667	284754	9.72%	1.076%
23	11.063	1555	1560	1565	rBV	105751	88326	3.01%	0.334%
24	11.239	1584	1590	1596	rBV3	83840	104310	3.56%	0.394%
25	11.310	1599	1602	1608	rVB	28217	29920	1.02%	0.113%
26	11.486	1628	1632	1635	rBV	36992	34449	1.18%	0.130%
27	11.516	1635	1637	1639	rBV	44100	35871	1.22%	0.136%
28	11.545	1639	1642	1644	rVV	56500	51322	1.75%	0.194%
29	11.598	1648	1651	1653	rBV	60434	54782	1.87%	0.207%
30	12.051	1723	1728	1734	rBV2	141970	159961	5.46%	0.605%
31	12.192	1748	1752	1756	rBV	520437	423260	14.44%	1.600%
32	12.416	1785	1790	1793	rBV	398615	392738	13.40%	1.484%
33	12.574	1813	1817	1820	rVB	1772596	1721178	58.73%	6.505%
34	12.751	1844	1847	1851	rVB	46207	45739	1.56%	0.173%

LSC Area Percent Report

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Misc :
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Instrument : BNA_F
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Integrator: RTE
Smoothing : ON Filtering: 5
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Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.816	1853	1858	1861	rVV2	29102	30726	1.05%	0.116%
36	13.045	1892	1897	1899	rBV5	21175	30409	1.04%	0.115%
37	13.363	1946	1951	1953	rBV	35707	36452	1.24%	0.138%
38	13.480	1966	1971	1977	rBV3	89533	142563	4.86%	0.539%
39	13.610	1985	1993	1996	rBV2	675651	814285	27.79%	3.078%
40	13.633	1996	1997	2001	rVB	148090	113698	3.88%	0.430%
41	13.874	2035	2038	2041	rBV5	19973	32011	1.09%	0.121%
42	14.092	2069	2075	2077	rBV5	29797	53126	1.81%	0.201%
43	14.468	2136	2139	2142	rBV3	27245	30069	1.03%	0.114%
44	14.604	2158	2162	2165	rBV	156306	214249	7.31%	0.810%
45	14.692	2174	2177	2181	rBV2	47576	47630	1.63%	0.180%
46	14.857	2201	2205	2210	rVB	81570	93852	3.20%	0.355%
47	14.910	2210	2214	2218	rVB	119423	140768	4.80%	0.532%
48	14.963	2218	2223	2229	rBV	457959	554635	18.93%	2.096%
49	16.180	2425	2430	2435	rBV	58968	102966	3.51%	0.389%
50	16.545	2487	2492	2496	rBV2	41612	70550	2.41%	0.267%
51	18.104	2755	2757	2763	rBV7	20135	34671	1.18%	0.131%

Sum of corrected areas: 26459100

LSC Report - Integrated Chromatogram

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Misc :
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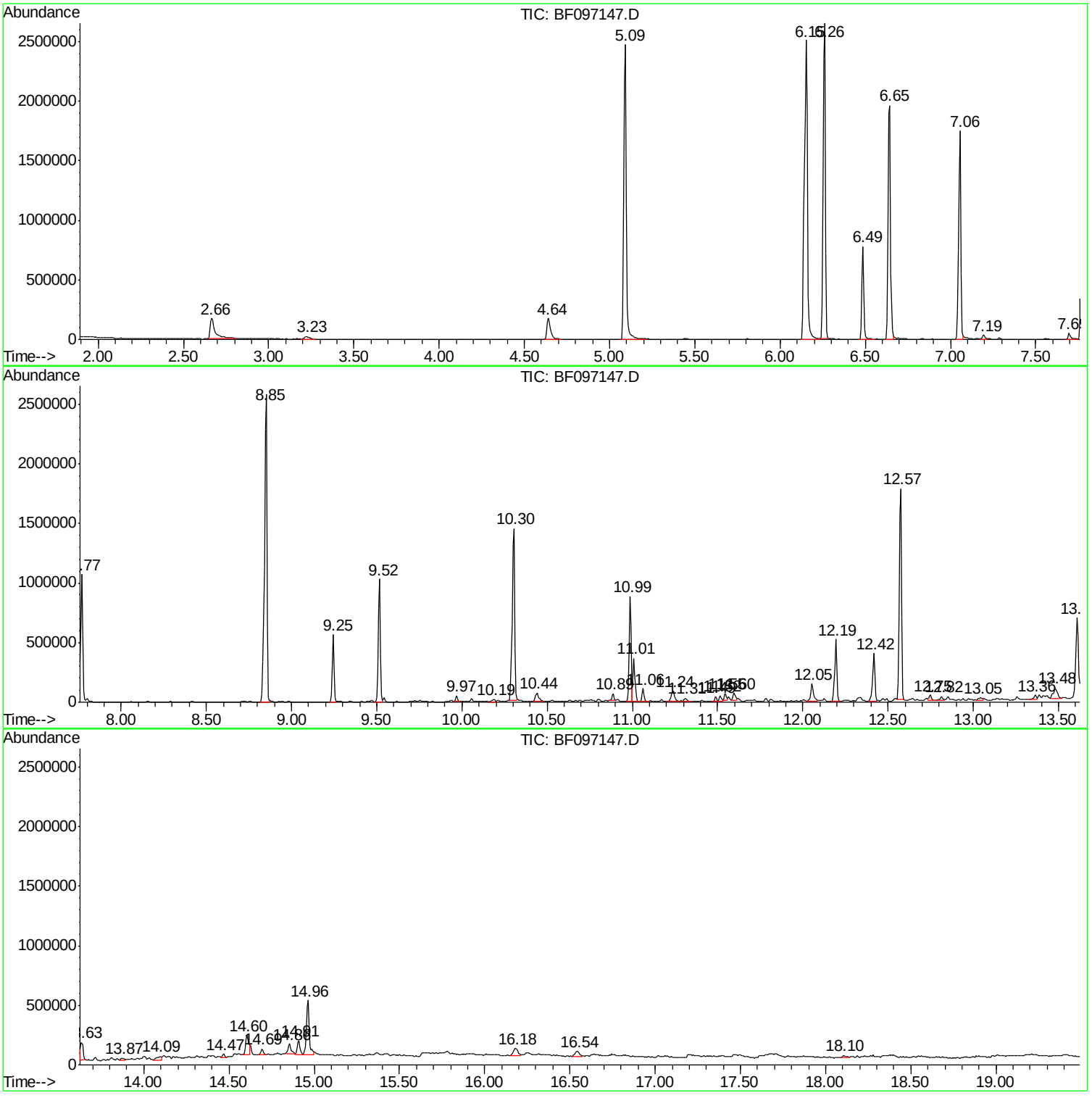
Instrument : BNA_F
ClientSampleId : T-1A-14.5-15.0-072117

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 : BF097147.D
Acq On : 28 Jul 2017 11:52
Operator : SJ/JU
Sample : I4397-01
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Instrument : BNA_F
ClientSampleId : T-1A-14.5-15.0-072117

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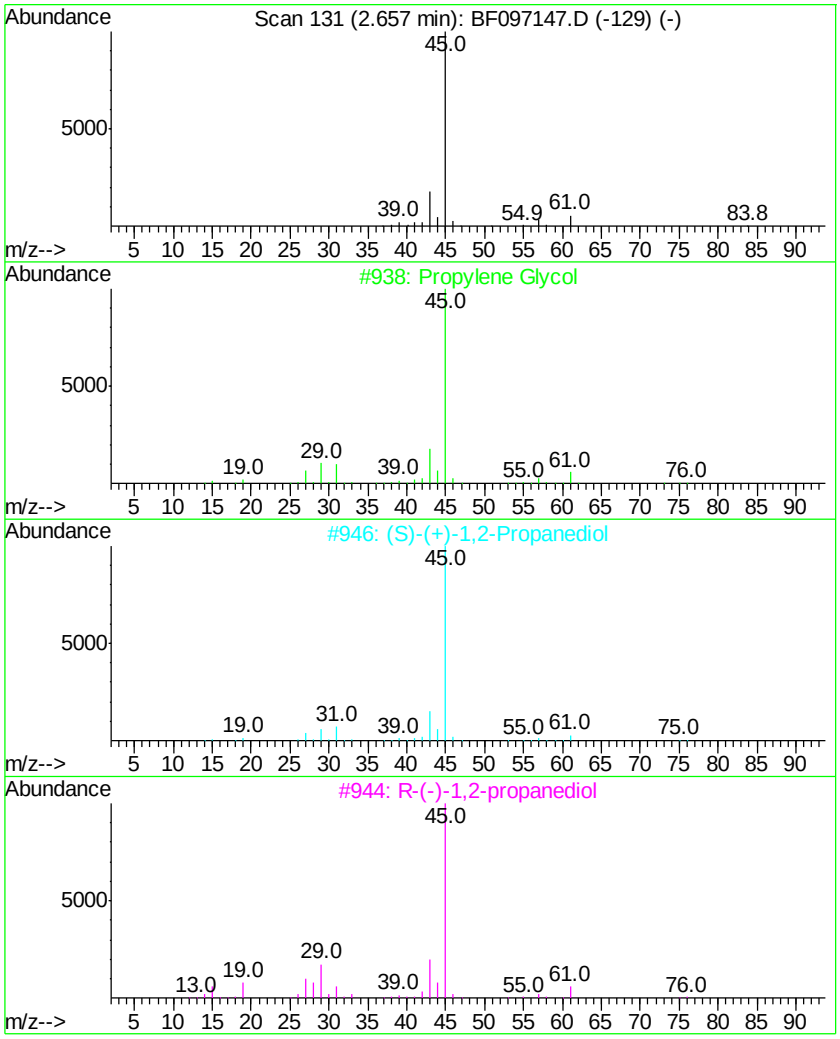
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

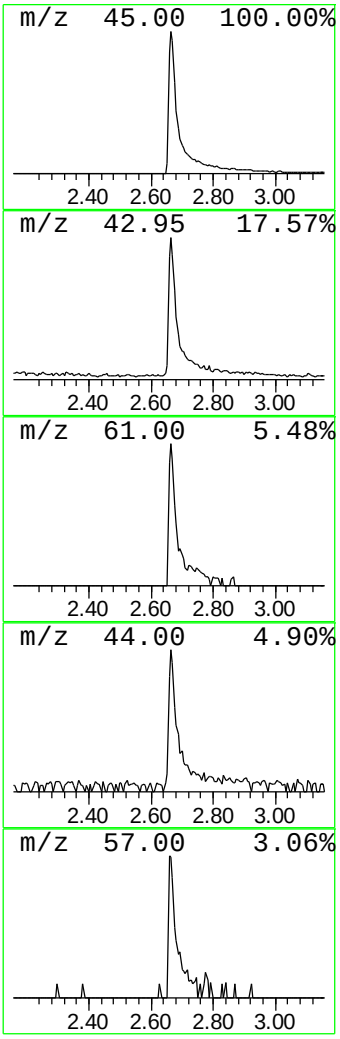
****

Peak Number 1 Propylene Glycol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.66	11.09 ng	372311	1,4-Dichlorobenzene-d4	6.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	74
2	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	64
3	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	9
4	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	002155-30-8	9
5	Formamide	45	CH3NO	000075-12-7	7





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Operator : SJ/JU
Sample : I4397-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T-1A-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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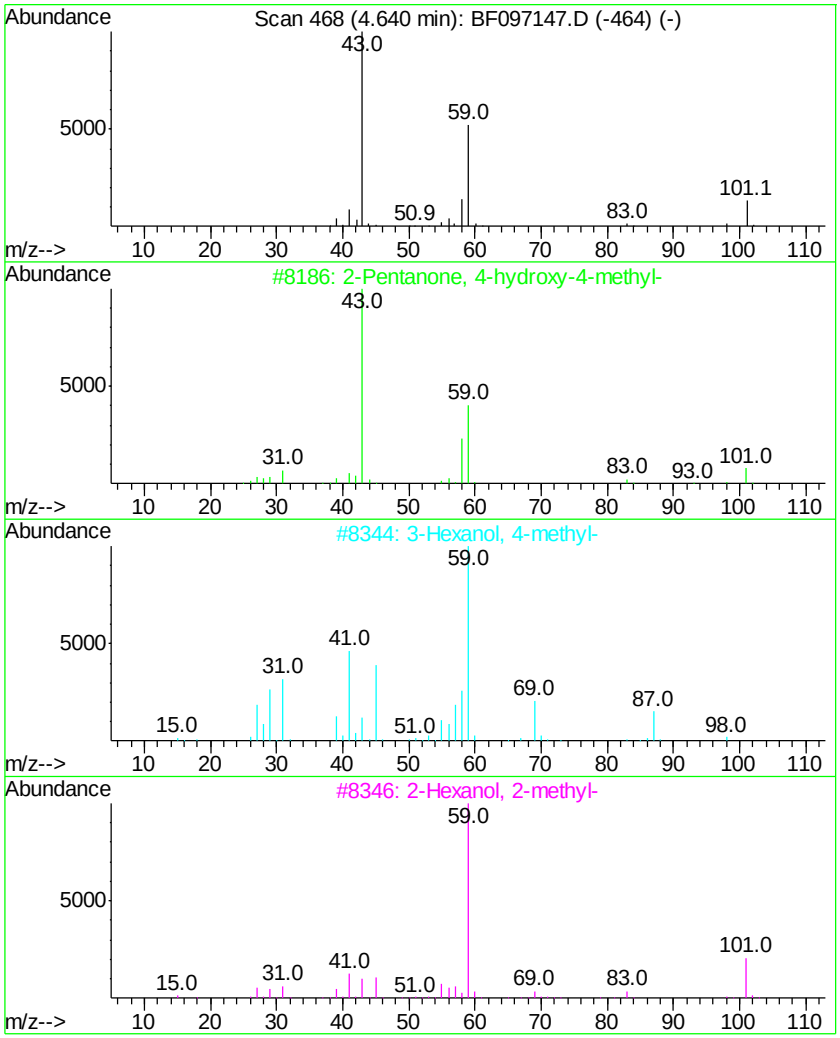
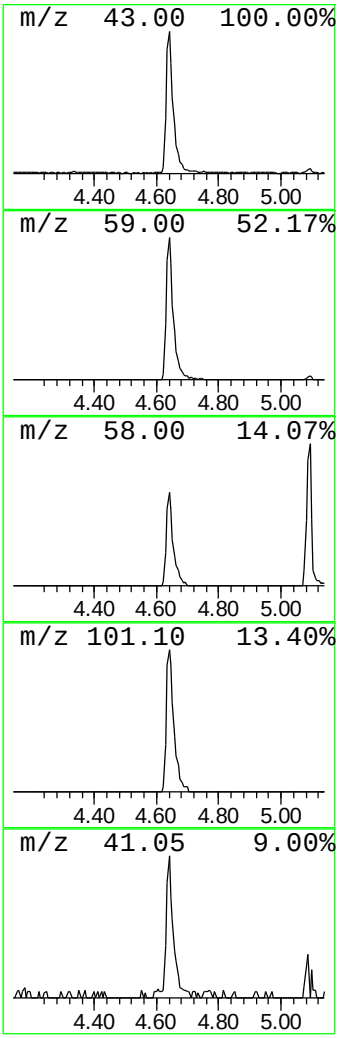
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.64	8.33 ng	279642	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	56
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	9
5	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	9





Library Search Compound Report

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Acq On : 28 Jul 2017 11:52
Operator : SJ/JU
Sample : I4397-01
Misc :
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Instrument : BNA_F
ClientSampleId : T-1A-14.5-15.0-072117

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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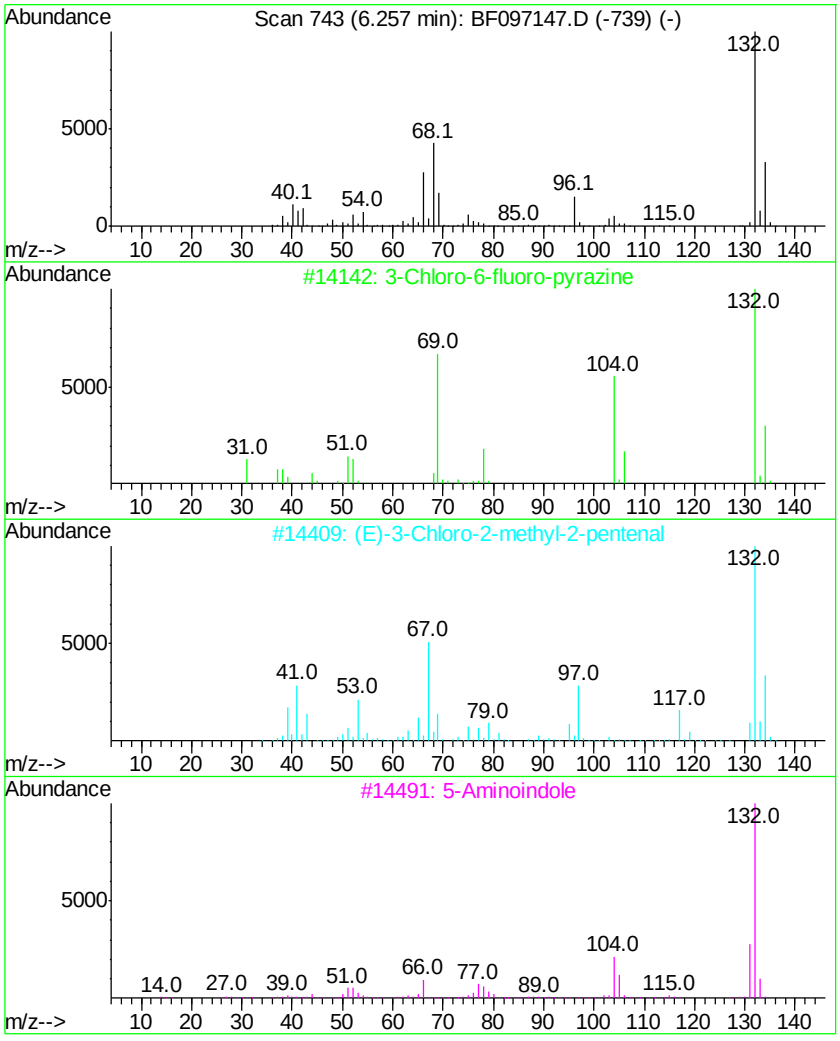
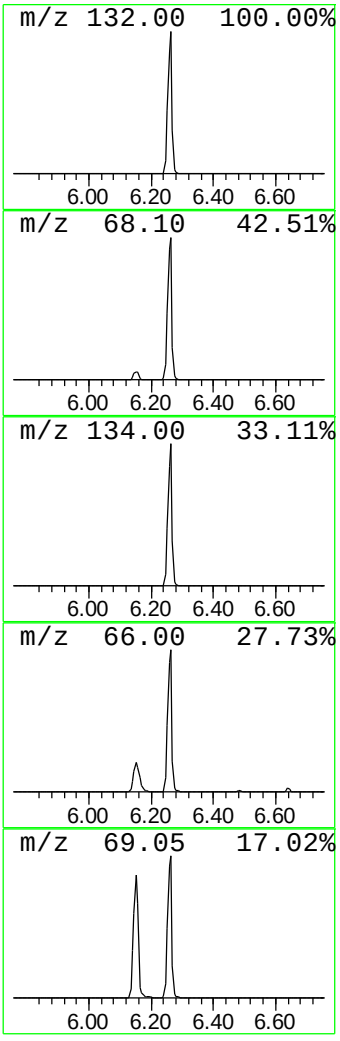
Peak Number 3 unknown6.26 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.26	76.54 ng	2569100	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	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9





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TIC Library : C:\DATABASE\NIST11.L
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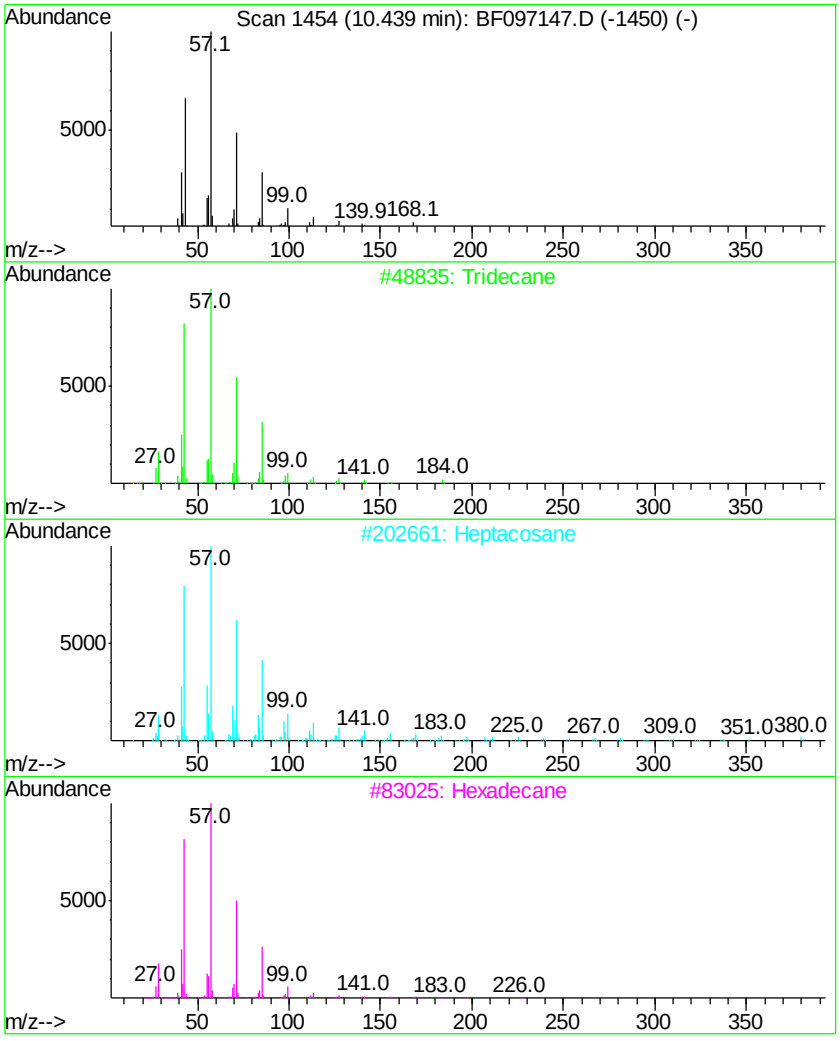
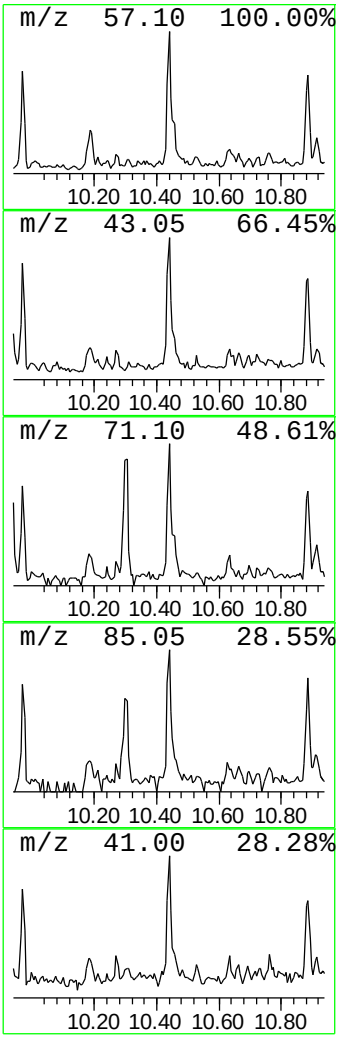
****

Peak Number 5 Tridecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.44	2.03 ng	78319	Phenanthrene-d10	10.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	90
2	Heptacosane	380	C27H56	000593-49-7	86
3	Hexadecane	226	C16H34	000544-76-3	86
4	Sulfurous acid, 2-propyl tetrade...	320	C17H36O3S	1000309-12-5	86
5	Sulfurous acid, butyl heptadecyl...	376	C21H44O3S	1000309-18-4	86





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

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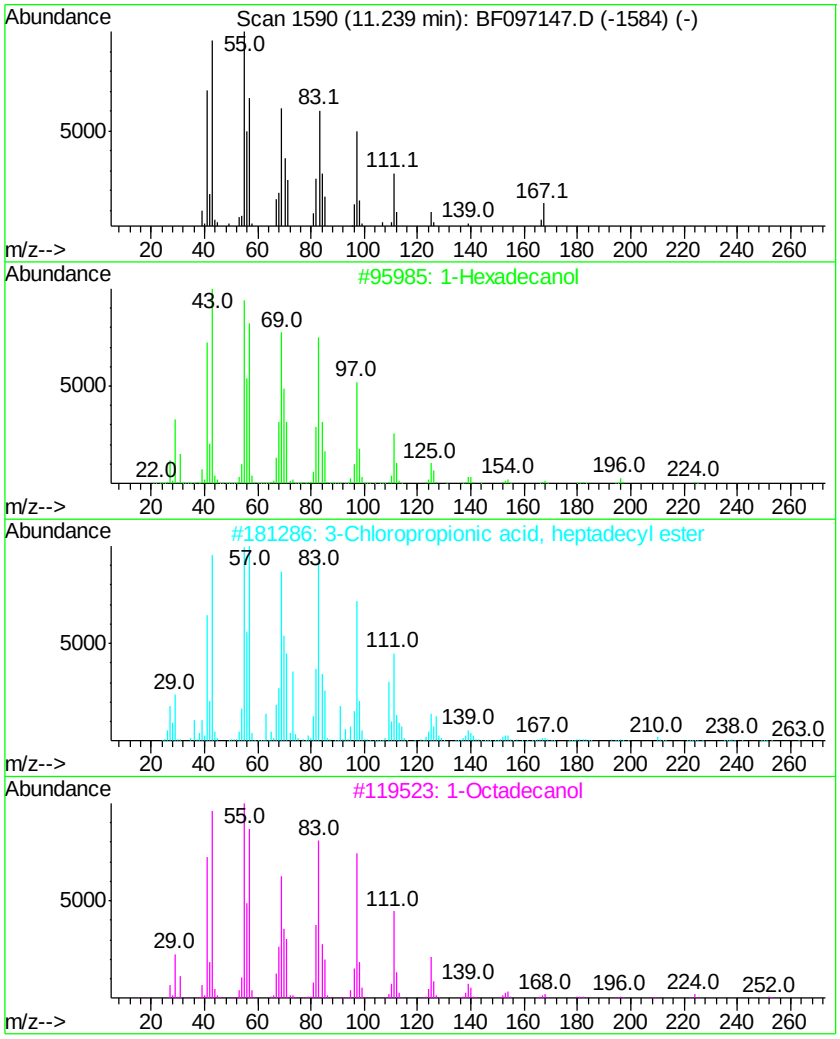
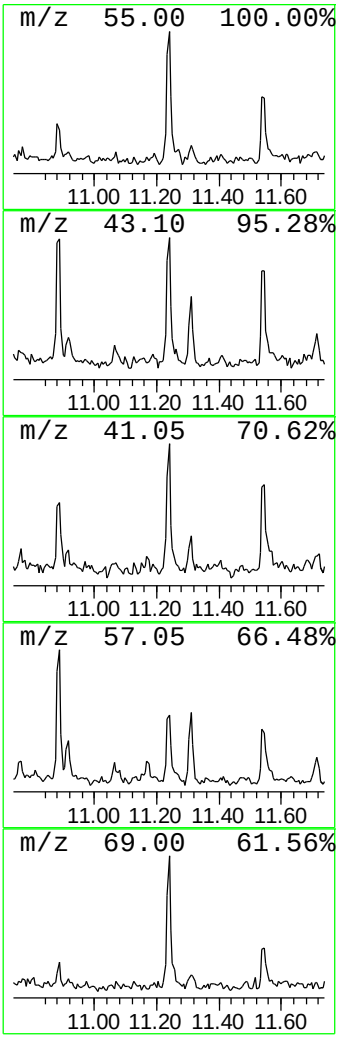
Peak Number 7 1-Hexadecanol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.24	2.70 ng	104310	Phenanthrene-d10	10.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexadecanol	242	C16H34O	036653-82-4	91
2	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	91
3	1-Octadecanol	270	C18H38O	000112-92-5	90
4	5-Eicosene, (E)-	280	C20H40	074685-30-6	90
5	Pentafluoropropionic acid, undec...	318	C14H23F5O2	959014-11-0	90





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

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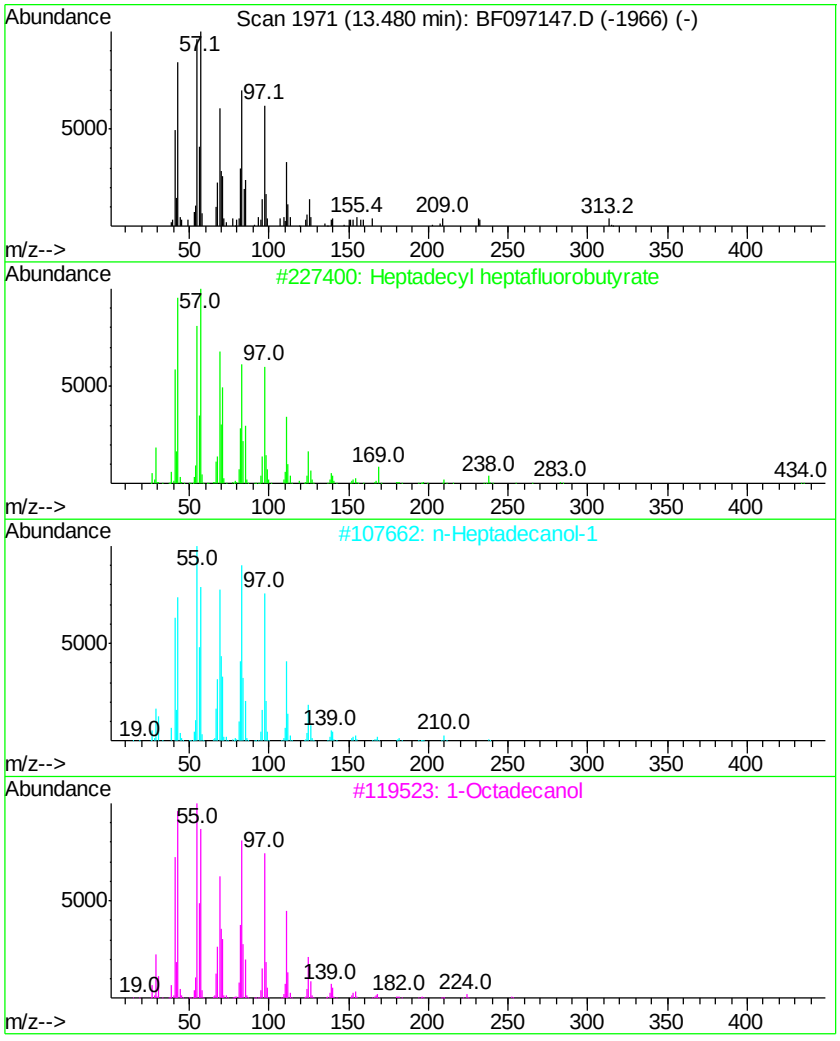
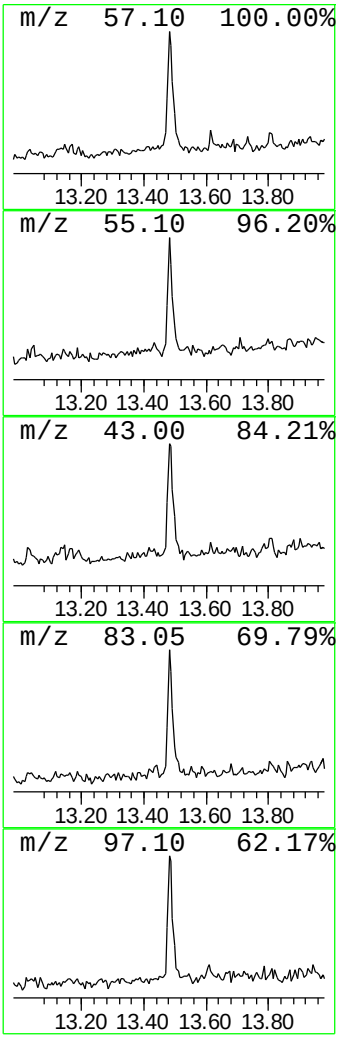
Peak Number 9 Heptadecyl heptafluorobutyrate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.48	3.50 ng	142563	Chrysene-d12	13.61

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
2	n-Heptadecanol-1	256	C17H36O	001454-85-9	90
3	1-Octadecanol	270	C18H38O	000112-92-5	90
4	1-Dodecanol, 2-octyl-, acetate	340	C22H44O2	074051-84-6	90
5	1-Hexadecanol	242	C16H34O	036653-82-4	87





Tentatively Identified Compound (LSC) summary

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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
Propylene Glycol	2.66	11.1	ng	372311	1	6.49	671269	20.0
2-Pentanone, 4-hy...	4.64	8.3	ng	279642	1	6.49	671269	20.0
unknown6.26	6.26	76.5	ng	2569100	1	6.49	671269	20.0
Tridecane	10.44	2.0	ng	78319	4	10.99	772275	20.0
1-Hexadecanol	11.24	2.7	ng	104310	4	10.99	772275	20.0
Heptadecyl heptaf...	13.48	3.5	ng	142563	5	13.61	814285	20.0