LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072817\
Data File : BF097149.D
Acq On : 28 Jul 2017 12:47
Operator : SJ/JU
Sample : I4397-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P-1A-4.0-4.5-072117

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	126	132	147	rBV	243696	576760	19.97%	2.161%
2	4.634	464	467	479	rBV	172431	296816	10.28%	1.112%
3	5.093	540	545	562	rBV	2489963	2876655	99.59%	10.777%
4	6.151	720	725	739	rBV	2293711	2888369	100.00%	10.821%
5	6.263	739	744	747	rBV	2654472	2552029	88.36%	9.561%
6	6.487	778	782	786	rBV	837190	699462	24.22%	2.620%
7	6.645	804	809	812	rBV	2071816	1989965	68.90%	7.455%
8	7.057	874	879	882	rBV	1898312	1794055	62.11%	6.721%
9	7.192	899	902	911	rVB	41643	52789	1.83%	0.198%
10	7.692	984	987	994	rBV	59955	61949	2.14%	0.232%
11	7.769	996	1000	1004	rBV	1218195	1026645	35.54%	3.846%
12	8.216	1072	1076	1083	rVB2	32905	36037	1.25%	0.135%
13	8.386	1098	1105	1108	rBV	50636	53696	1.86%	0.201%
14	8.851	1179	1184	1187	rBV	2878121	2734452	94.67%	10.244%
15	8.945	1198	1200	1204	rVB	101385	80089	2.77%	0.300%
16	9.245	1248	1251	1254	rBV	554213	442952	15.34%	1.659%
17	9.475	1286	1290	1292	rVB	125707	111935	3.88%	0.419%
18	9.516	1292	1297	1301	rBV	1046669	962942	33.34%	3.608%
19	9.710	1323	1330	1332	rBV7	25335	47740	1.65%	0.179%
20	9.757	1335	1338	1342	rVV3	26961	38712	1.34%	0.145%
21	9.792	1342	1344	1347	rVB	56025	44875	1.55%	0.168%
22	9.828	1347	1350	1353	rBV2	28820	32125	1.11%	0.120%
23	9.969	1371	1374	1377	rVB	201417	156639	5.42%	0.587%
24	10.192	1406	1412	1414	rBV	101627	123386	4.27%	0.462%
25	10.304	1427	1431	1435	rBV	1332491	1334116	46.19%	4.998%
26	10.439	1450	1454	1455	rBV	233454	196264	6.79%	0.735%
27	10.633	1484	1487	1490	rBV3	62955	71516	2.48%	0.268%
28	10.722	1500	1502	1506	rBV3	30356	42031	1.46%	0.157%
29	10.886	1527	1530	1532	rBV	162667	125123	4.33%	0.469%
30	10.916	1532	1535	1541	rVB	117145	117079	4.05%	0.439%
31	10.986	1543	1547	1550	rBV	857700	743858	25.75%	2.787%
32	11.010	1550	1551	1555	rVV2	47076	42872	1.48%	0.161%
33	11.063	1558	1560	1564	rVB2	29401	32646	1.13%	0.122%
34	11.263	1592	1594	1597	rVB	33085	30094	1.04%	0.113%

LSC Area Percent Report

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Data File : BF097149.D
Acq On : 28 Jul 2017 12:47
Operator : SJ/JU
Sample : I4397-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P-1A-4.0-4.5-072117

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	11.310	1599	1602	1606	rVB	130800	110164	3.81%	0.413%
36	11.545	1639	1642	1644	rBV	86914	75643	2.62%	0.283%
37	11.598	1649	1651	1662	rVB10	42693	89257	3.09%	0.334%
38	11.716	1668	1671	1675	rVB	87303	85368	2.96%	0.320%
39	12.104	1734	1737	1739	rVB	48325	42168	1.46%	0.158%
40	12.192	1749	1752	1756	rVB	111230	102937	3.56%	0.386%
41	12.321	1771	1774	1779	rBV6	54501	100192	3.47%	0.375%
42	12.416	1787	1790	1793	rVB	106839	96977	3.36%	0.363%
43	12.469	1797	1799	1801	rBV	34420	30349	1.05%	0.114%
44	12.574	1812	1817	1820	rBV	1779917	1721677	59.61%	6.450%
45	13.168	1916	1918	1926	rVB7	26138	31285	1.08%	0.117%
46	13.410	1956	1959	1961	rBV3	27416	40834	1.41%	0.153%
47	13.480	1969	1971	1981	rVB	106820	154578	5.35%	0.579%
48	13.610	1989	1993	1997	rBV	659033	682039	23.61%	2.555%
49	14.504	2142	2145	2146	rBV2	40025	34905	1.21%	0.131%
50	14.604	2159	2162	2169	rVB	76191	118074	4.09%	0.442%
51	14.910	2211	2214	2218	rVB	39358	46834	1.62%	0.175%
52	14.962	2218	2223	2229	rBV	492798	568255	19.67%	2.129%
53	15.145	2250	2254	2255	rBV4	37153	51592	1.79%	0.193%
54	16.539	2488	2491	2500	rVB5	26919	52660	1.82%	0.197%
55	17.245	2607	2611	2612	rBV3	29901	40047	1.39%	0.150%

Sum of corrected areas: 26692508

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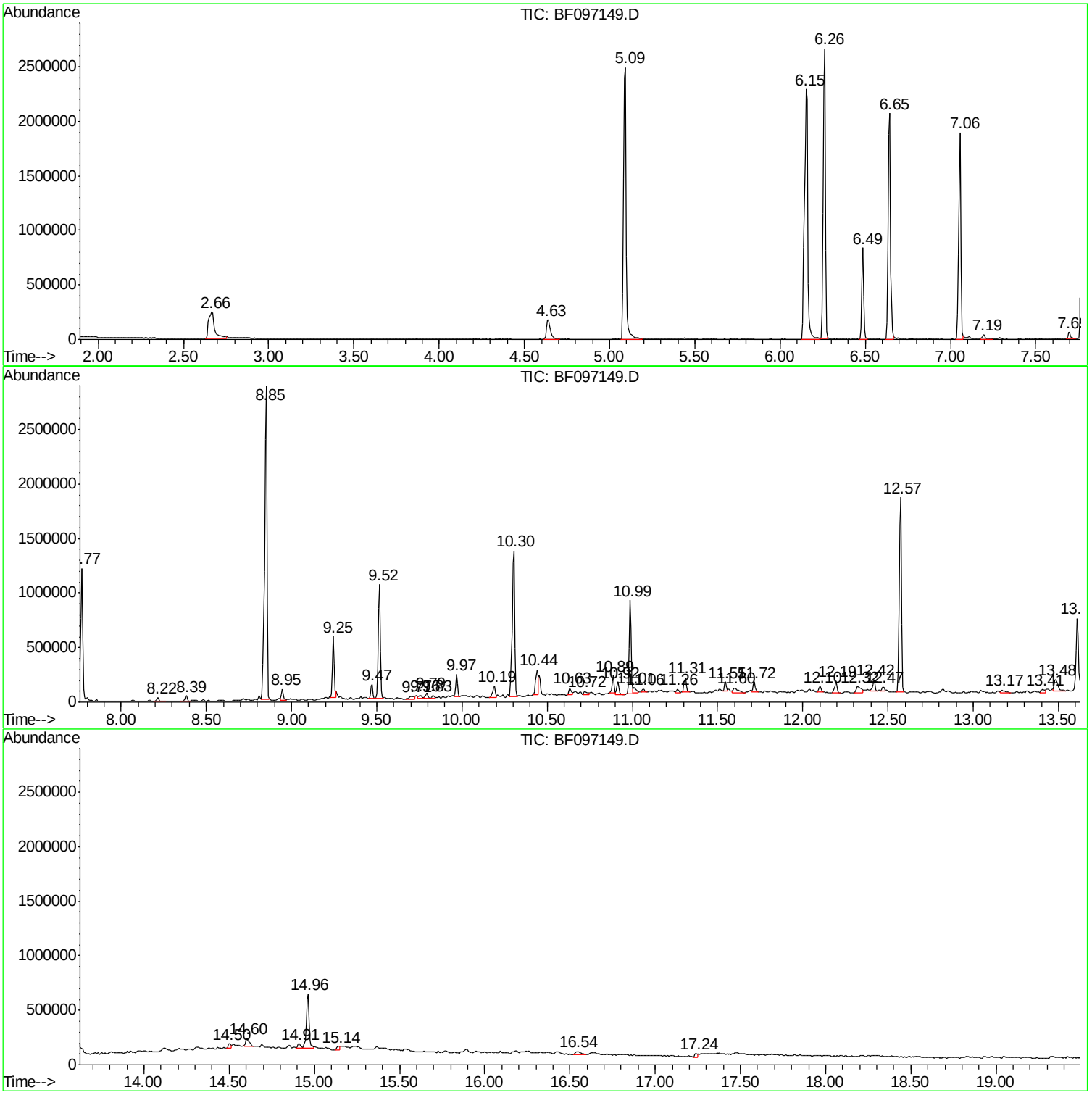
Instrument :
BNA_F
ClientSampleId :
P-1A-4.0-4.5-072117

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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Operator : SJ/JU
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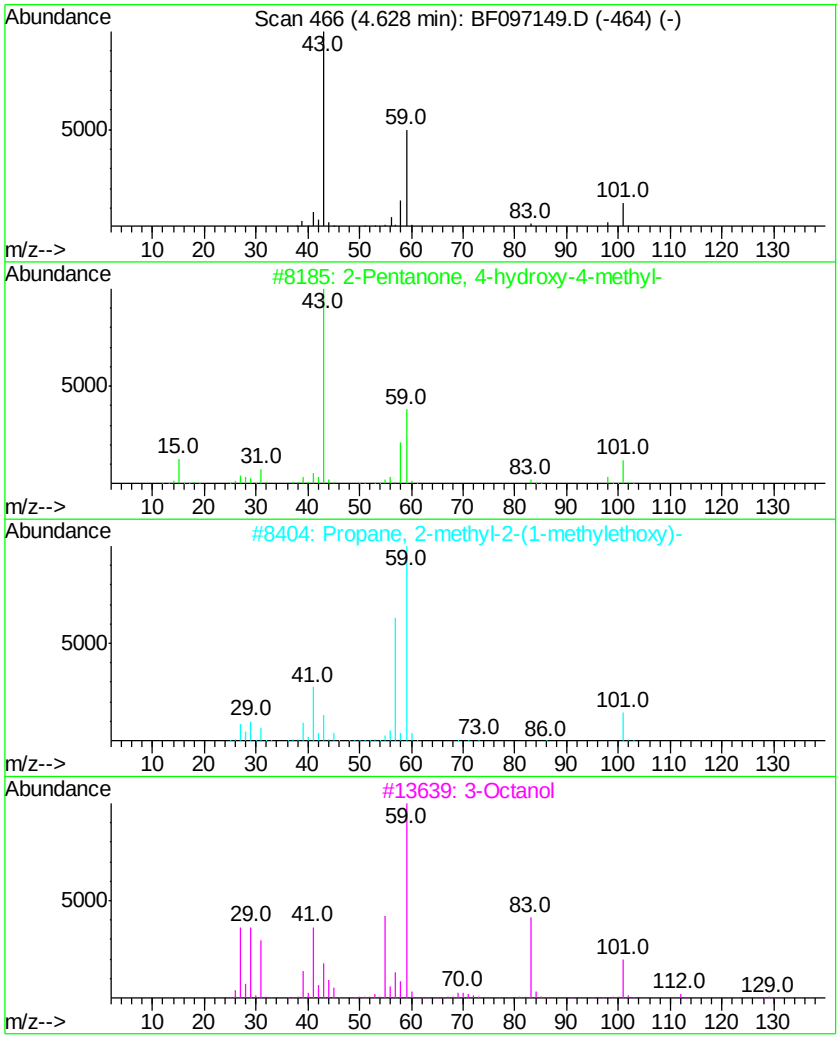
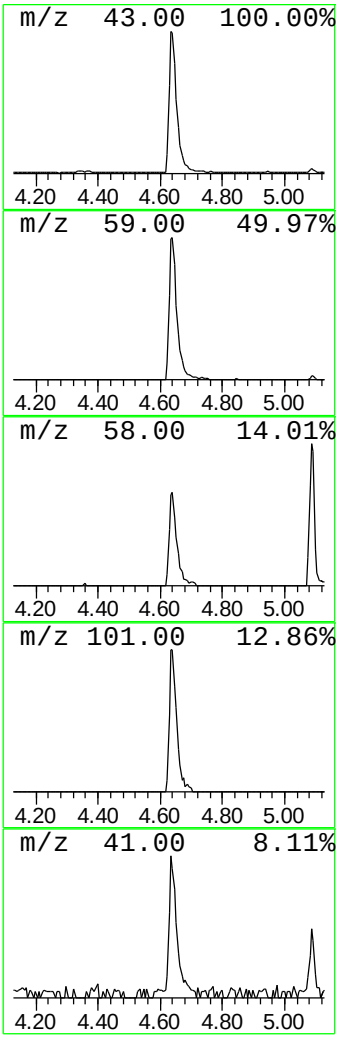
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.63	8.49 ng	296816	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	3-Octanol	130	C8H18O	000589-98-0	33
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5	Silane, dimethyl-	60	C2H8Si	001111-74-6	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF072817\
Data File : BF097149.D
Acq On : 28 Jul 2017 12:47
Operator : SJ/JU
Sample : I4397-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P-1A-4.0-4.5-072117

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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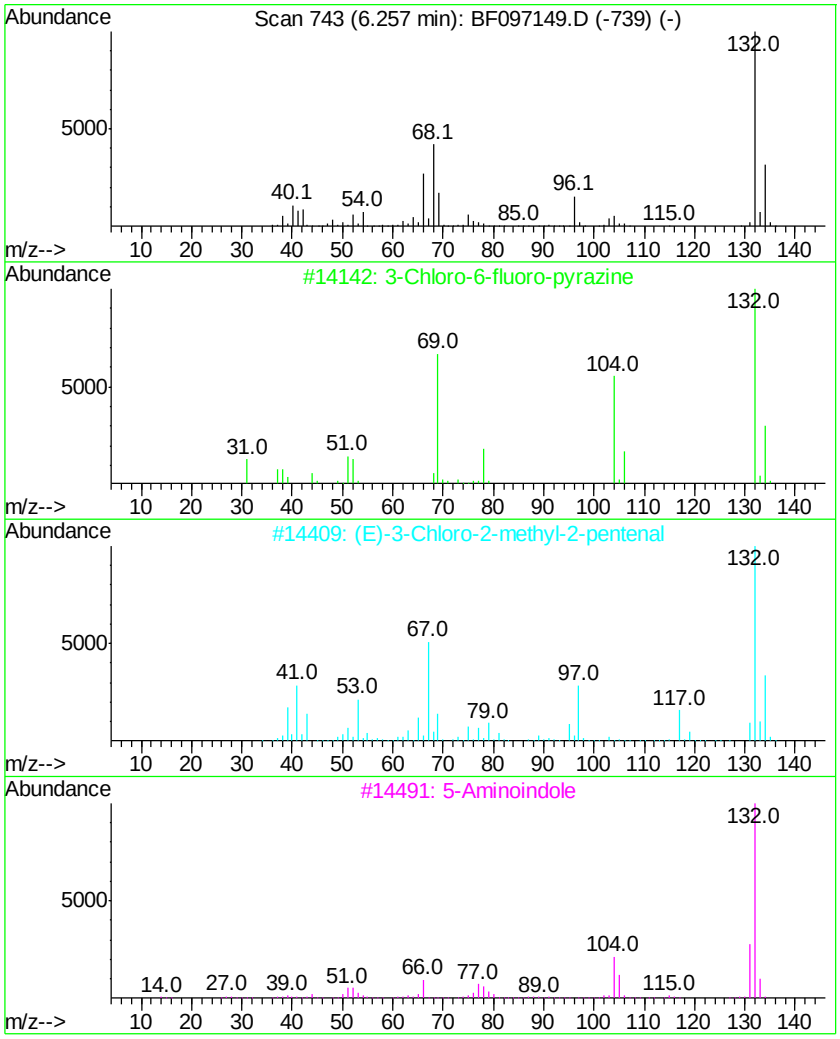
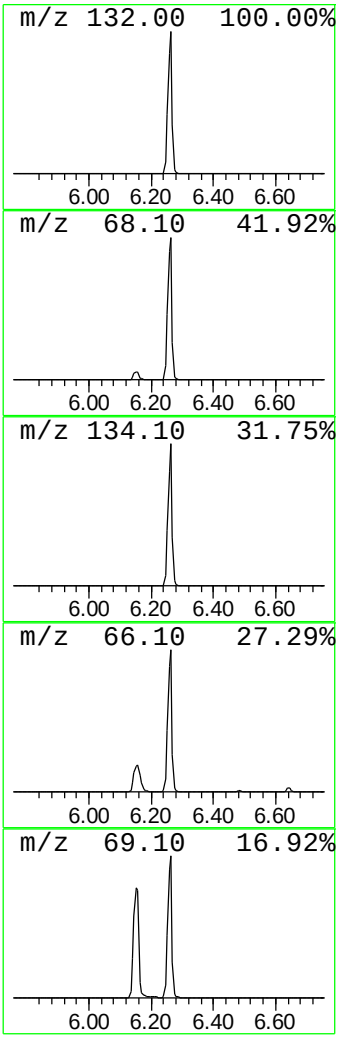
Peak Number 3 unknown6.26 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.26	72.97 ng	2552030	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	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072817\
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Operator : SJ/JU
Sample : I4397-03
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Instrument : BNA_F
ClientSampleId : P-1A-4.0-4.5-072117

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
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TIC Library : C:\DATABASE\NIST11.L
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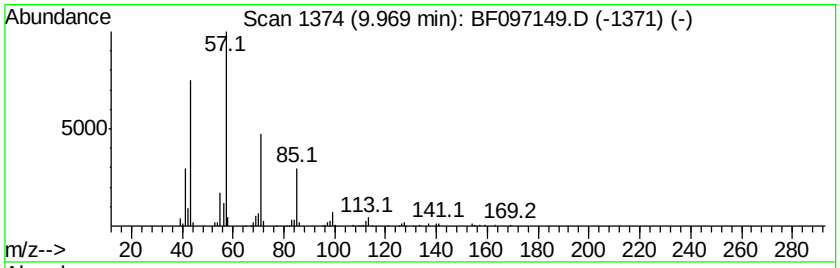
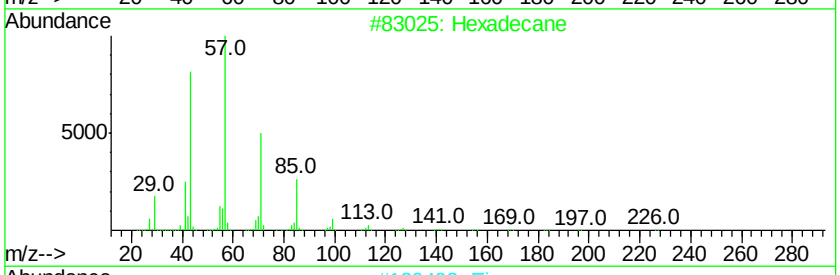
****

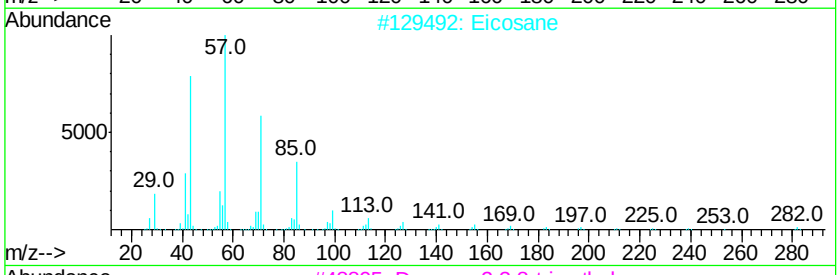
Peak Number 5 Hexadecane Concentration Rank 8

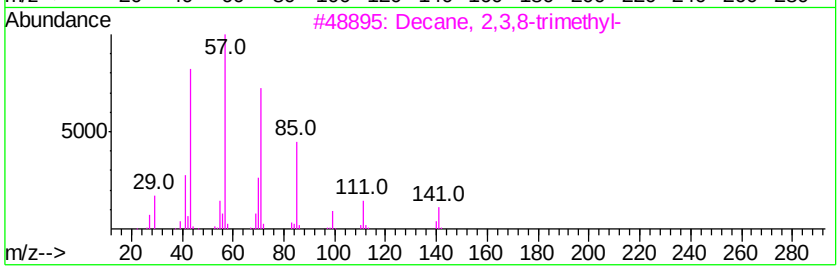
R.T.	EstConc	Area	Relative to ISTD	R.T.
9.97	3.25 ng	156639	Acenaphthene-d10	9.52

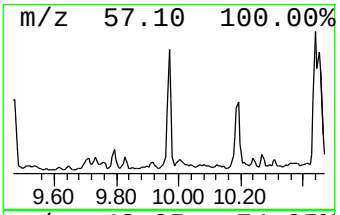
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	91
2	Eicosane	282	C20H42	000112-95-8	78
3	Decane, 2,3,8-trimethyl-	184	C13H28	062238-14-6	78
4	Tridecane	184	C13H28	000629-50-5	72
5	Nonane, 5-butyl-	184	C13H28	017312-63-9	64

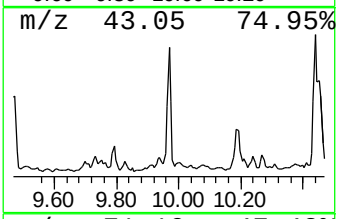


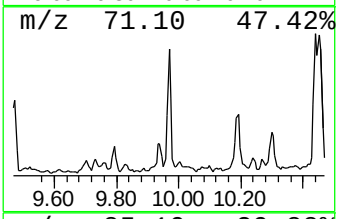


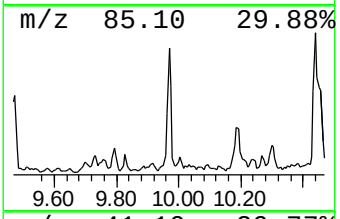


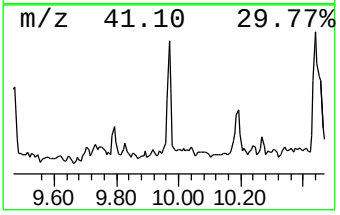












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ClientSampleId : P-1A-4.0-4.5-072117

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

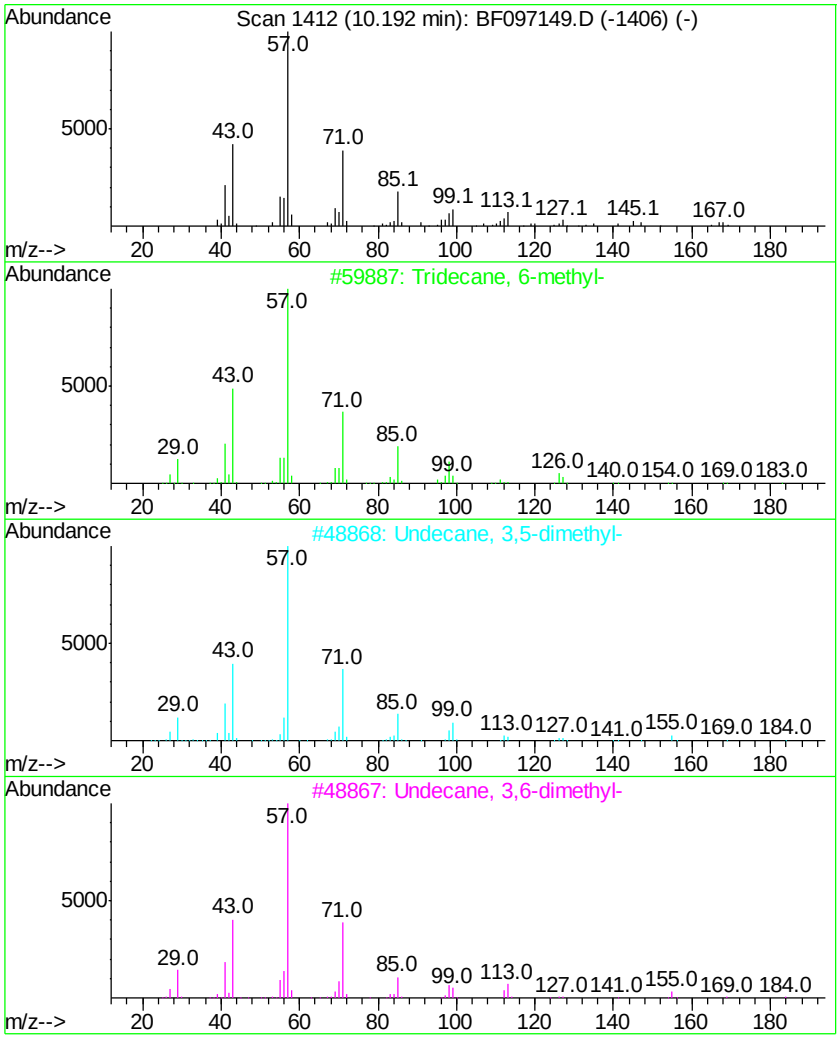
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

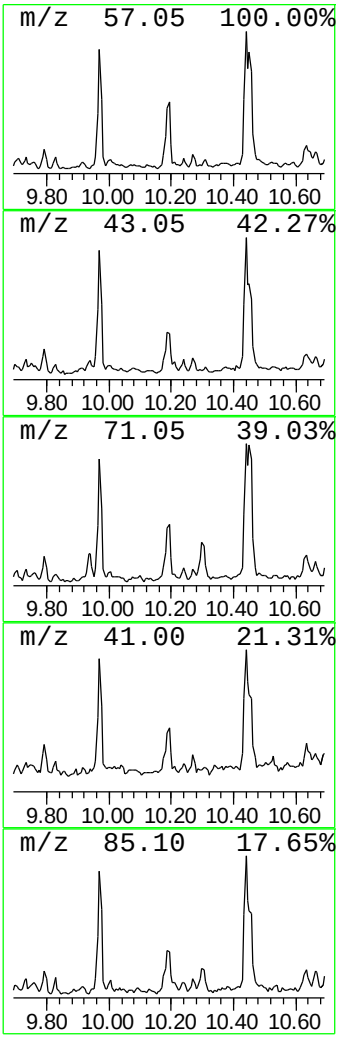
****

Peak Number 6 Tridecane, 6-methyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.19	2.56 ng	123386	Acenaphthene-d10	9.52

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane, 6-methyl-	198	C14H30	013287-21-3	80
2	Undecane, 3,5-dimethyl-	184	C13H28	017312-81-1	78
3	Undecane, 3,6-dimethyl-	184	C13H28	017301-28-9	78
4	Decane, 2,6,8-trimethyl-	184	C13H28	062108-26-3	72
5	Tetratetracontane	619	C44H90	007098-22-8	72





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Misc :
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Instrument : BNA_F
ClientSampleId : P-1A-4.0-4.5-072117

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

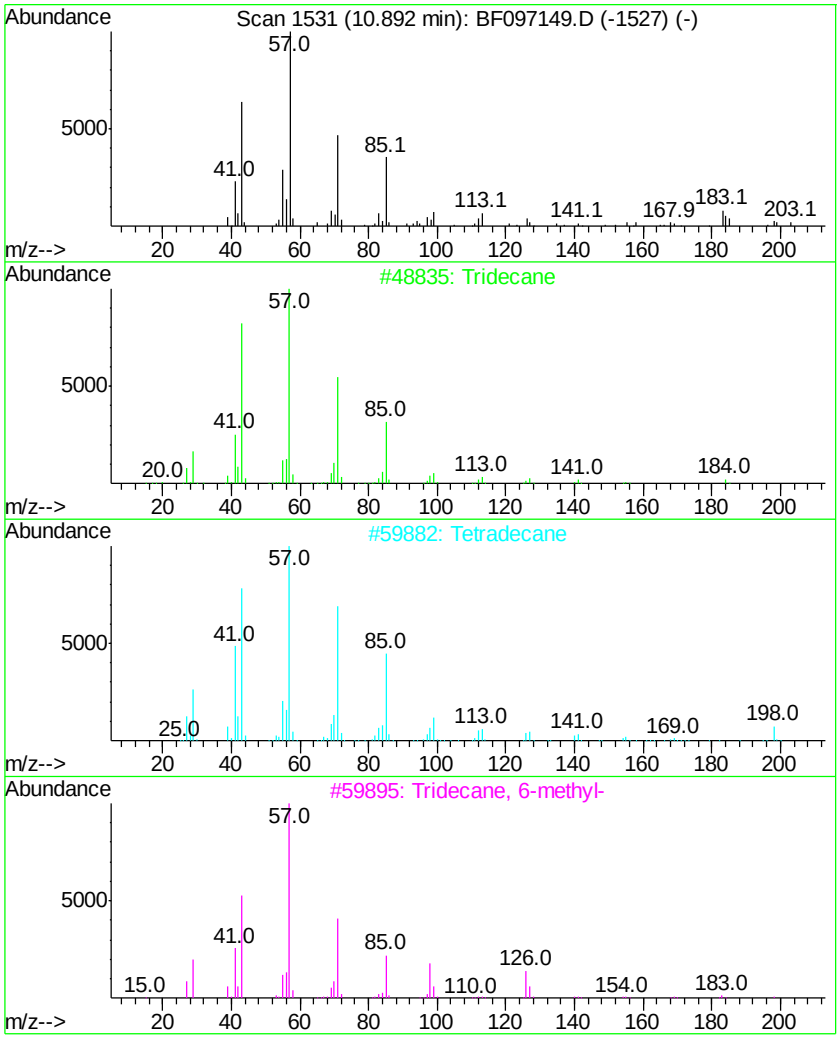
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

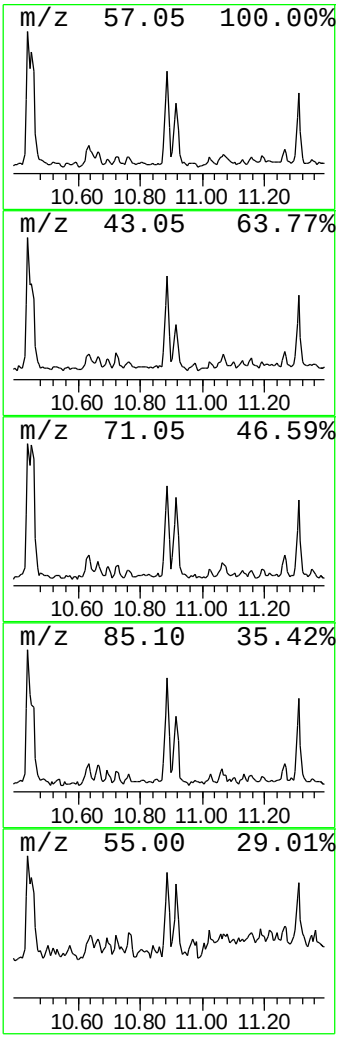
****

Peak Number 8 Tridecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.89	3.36 ng	125123	Phenanthrene-d10	10.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	95
2	Tetradecane	198	C14H30	000629-59-4	91
3	Tridecane, 6-methyl-	198	C14H30	013287-21-3	87
4	Heptadecane	240	C17H36	000629-78-7	80
5	Hexadecane	226	C16H34	000544-76-3	80





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Instrument : BNA_F
ClientSampleId : P-1A-4.0-4.5-072117

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

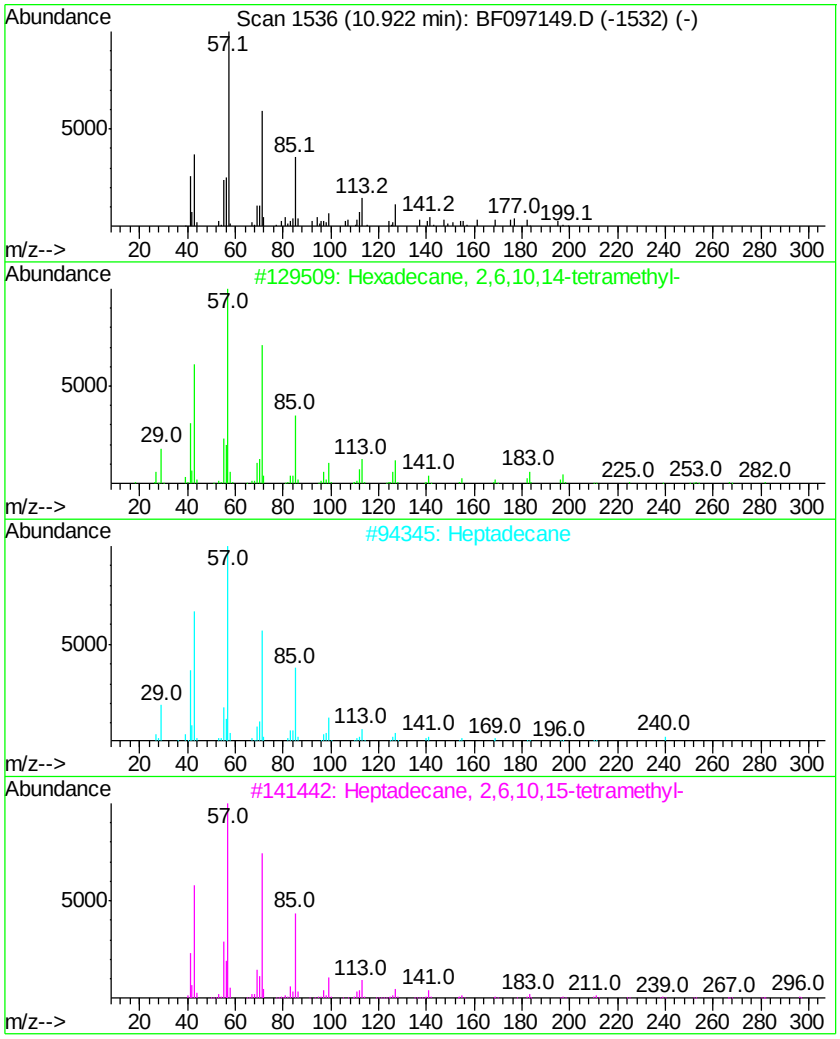
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

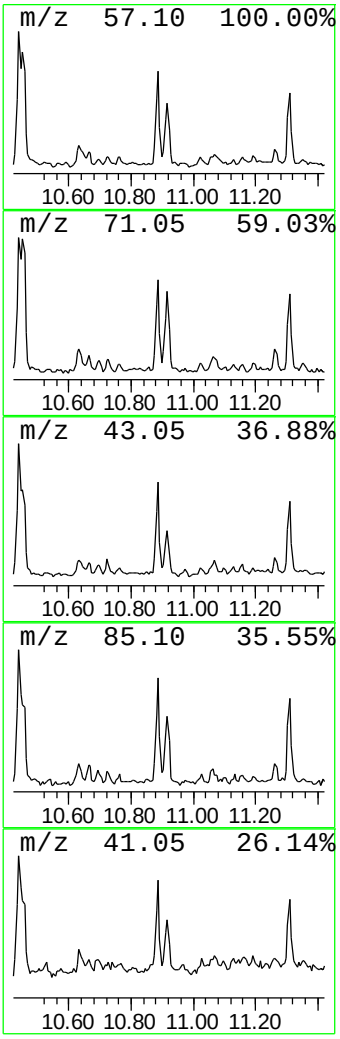
****

Peak Number 9 Hexadecane, 2,6,10,14-tetra... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.92	3.15 ng	117079	Phenanthrene-d10	10.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	91
2	Heptadecane	240	C17H36	000629-78-7	90
3	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	86
4	Heptacosane	380	C27H56	000593-49-7	86
5	Decane, 2-methyl-	156	C11H24	006975-98-0	83





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Operator : SJ/JU
Sample : I4397-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P-1A-4.0-4.5-072117

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
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TIC Integration Parameters: LSCINT.P

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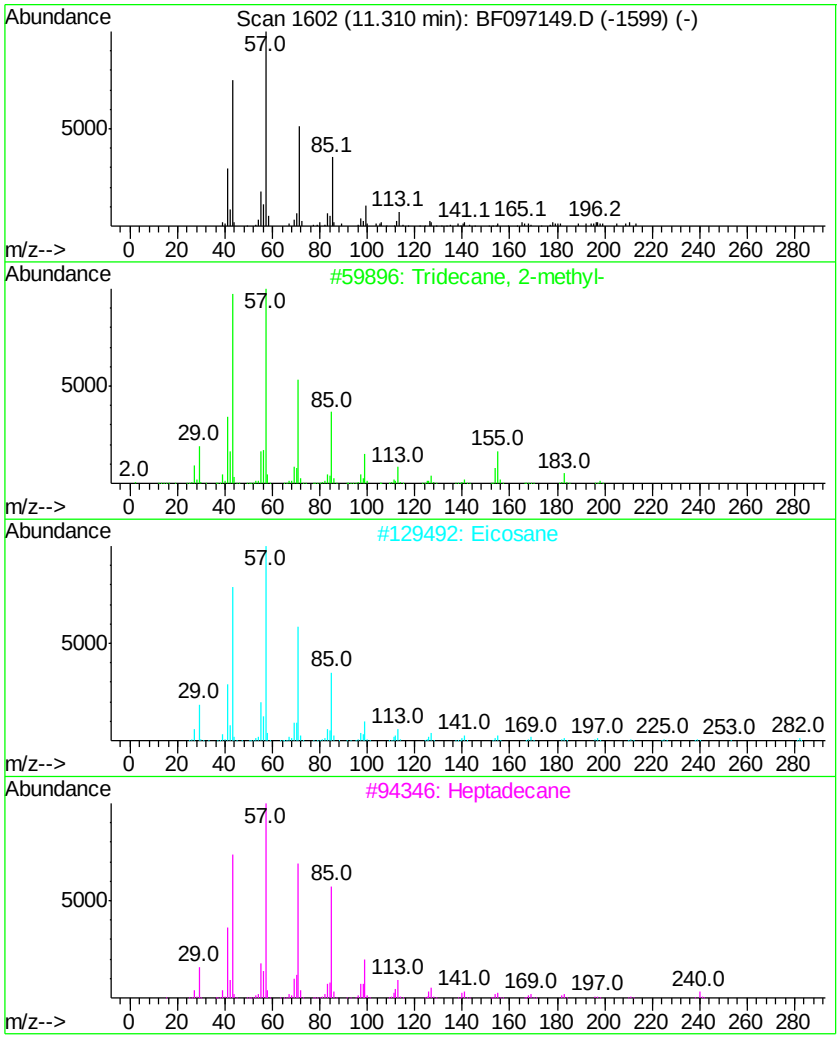
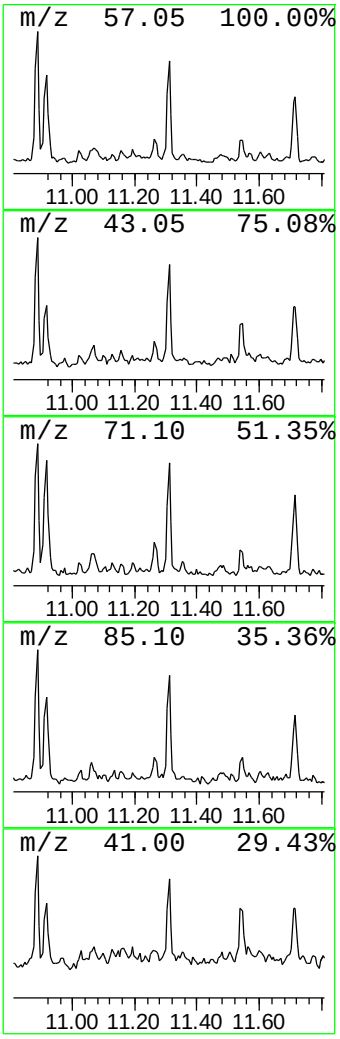
Peak Number 10 Tridecane, 2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.31	2.96 ng	110164	Phenanthrene-d10	10.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane, 2-methyl-	198	C14H30	001560-96-9	86
2	Eicosane	282	C20H42	000112-95-8	80
3	Heptadecane	240	C17H36	000629-78-7	72
4	Undecane, 2,9-dimethyl-	184	C13H28	017301-26-7	72
5	Decane, 2,3,8-trimethyl-	184	C13H28	062238-14-6	64





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Data File : BF097149.D
Acq On : 28 Jul 2017 12:47
Operator : SJ/JU
Sample : I4397-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P-1A-4.0-4.5-072117

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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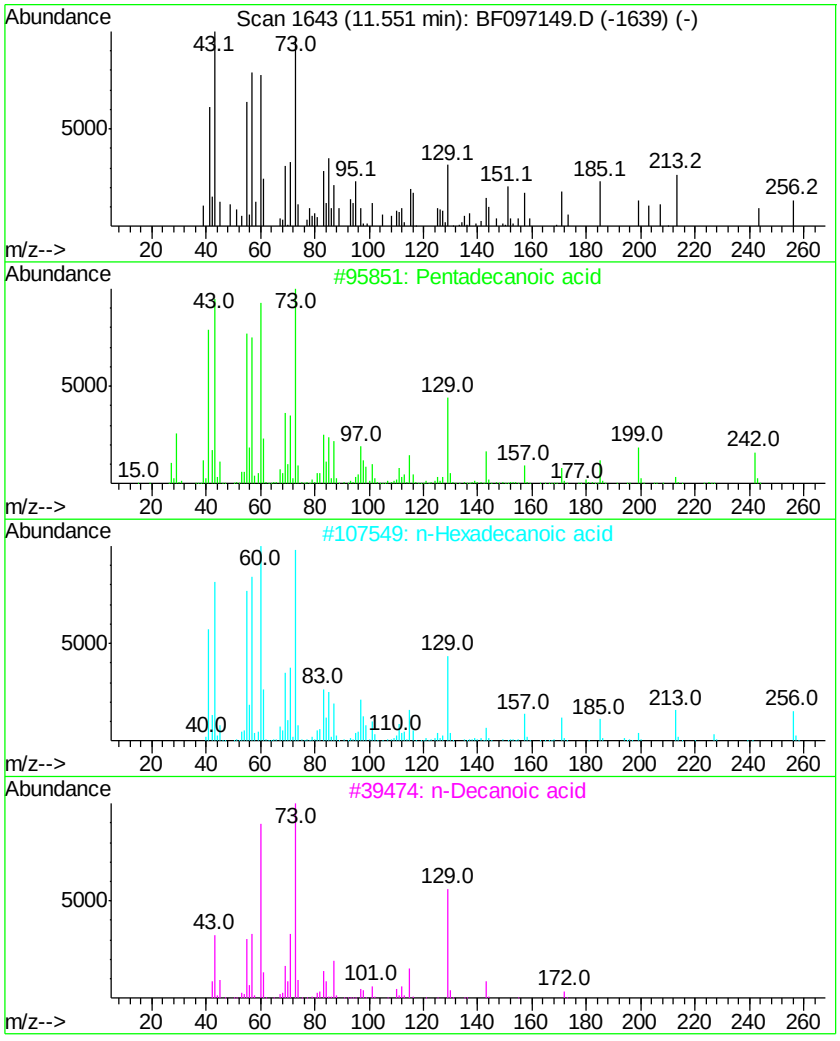
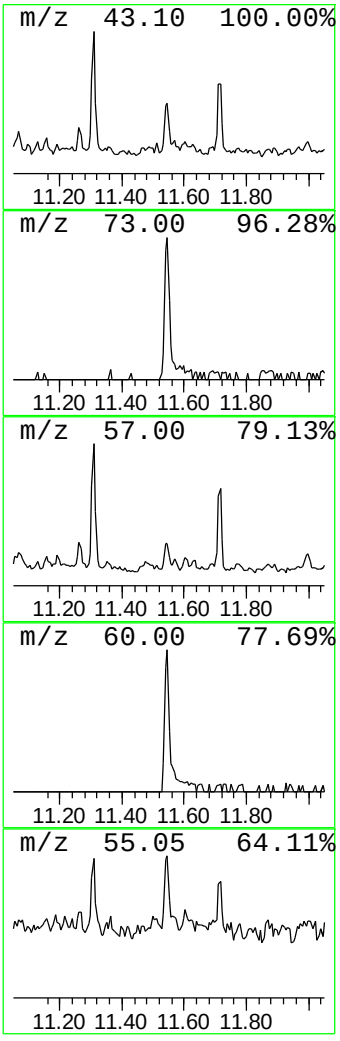
Peak Number 11 Pentadecanoic acid Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.55	2.03 ng	75643	Phenanthrene-d10	10.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	72
3	n-Decanoic acid	172	C10H20O2	000334-48-5	49
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	38
5	Heptanoic acid	130	C7H14O2	000111-14-8	35





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Sample : I4397-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P-1A-4.0-4.5-072117

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
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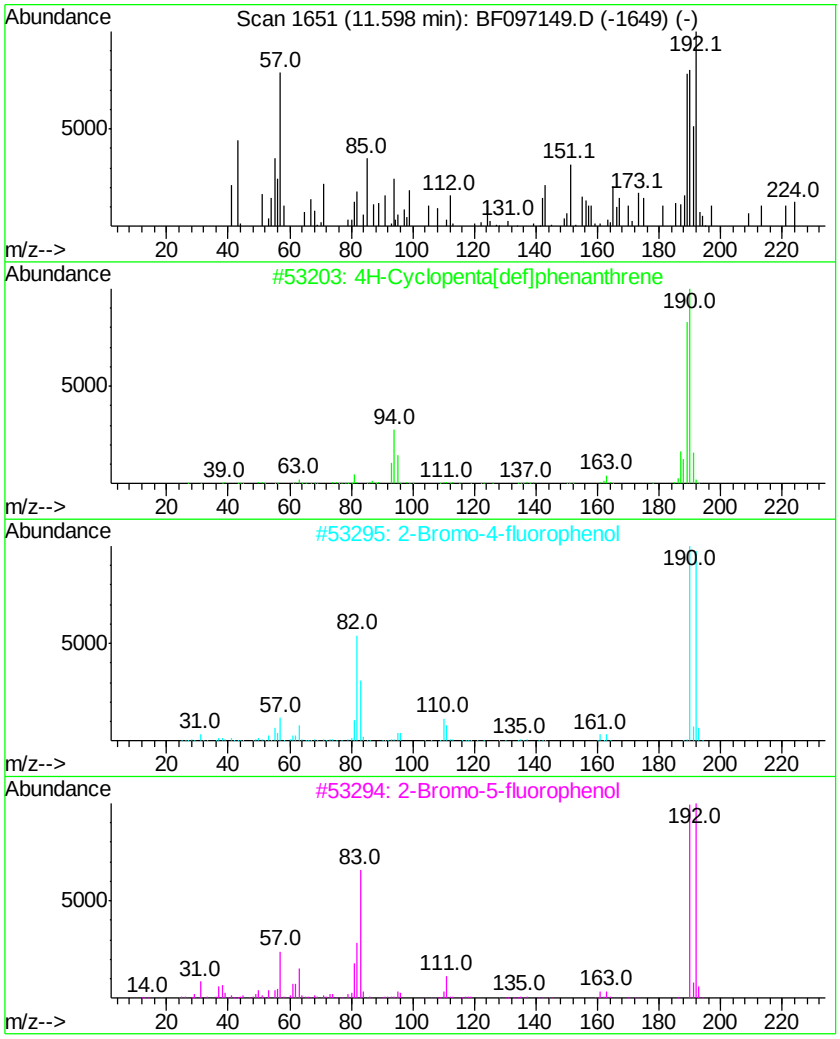
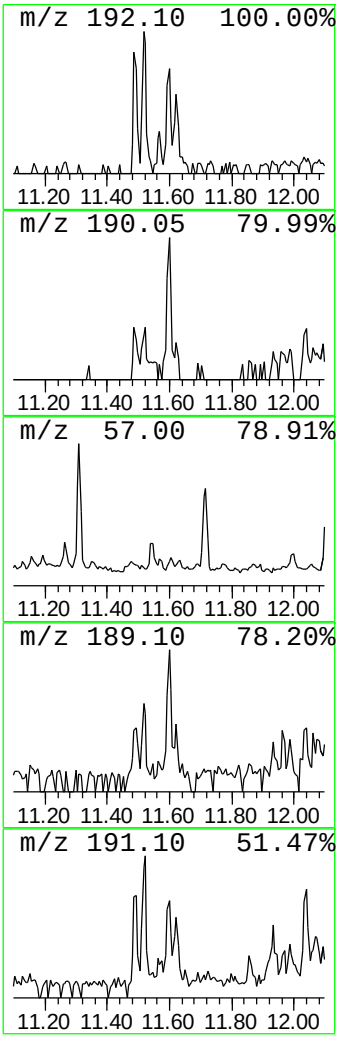
Peak Number 12 unknown11.60 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.60	2.40 ng	89257	Phenanthrene-d10	10.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	43
2	2-Bromo-4-fluorophenol	190	C6H4BrFO	000496-69-5	38
3	2-Bromo-5-fluorophenol	190	C6H4BrFO	147460-41-1	35
4	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	27
5	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	27





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Acq On : 28 Jul 2017 12:47
Operator : SJ/JU
Sample : I4397-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P-1A-4.0-4.5-072117

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
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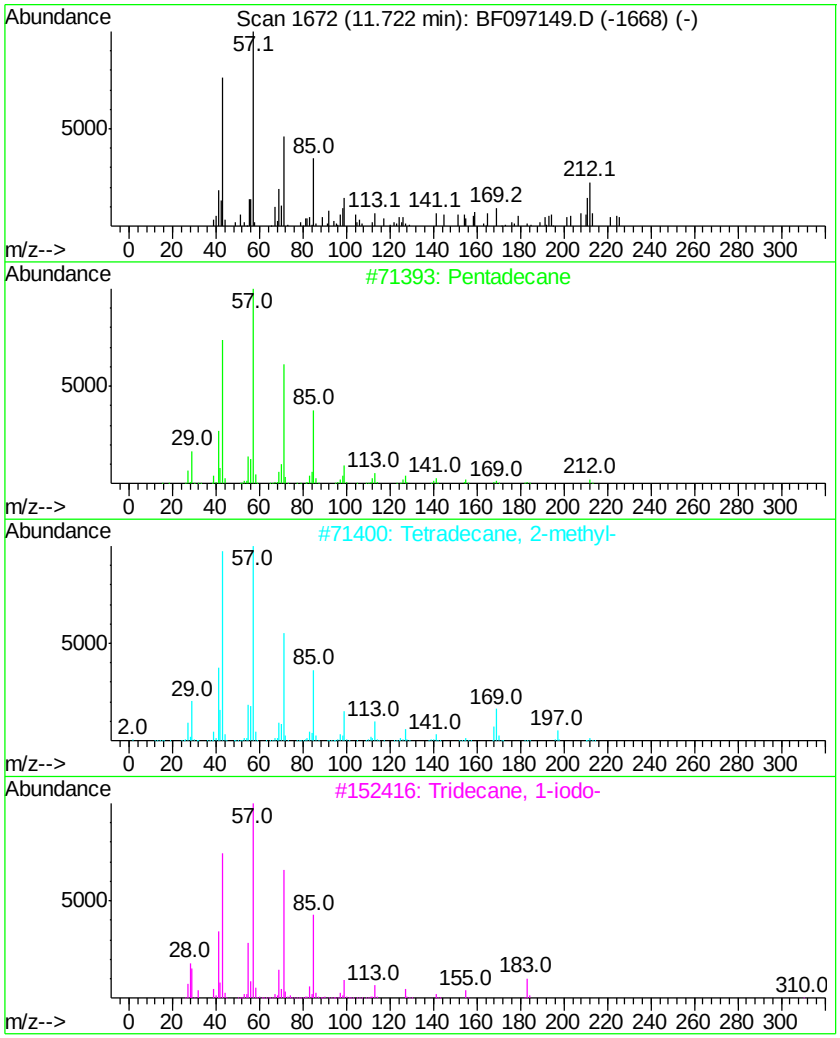
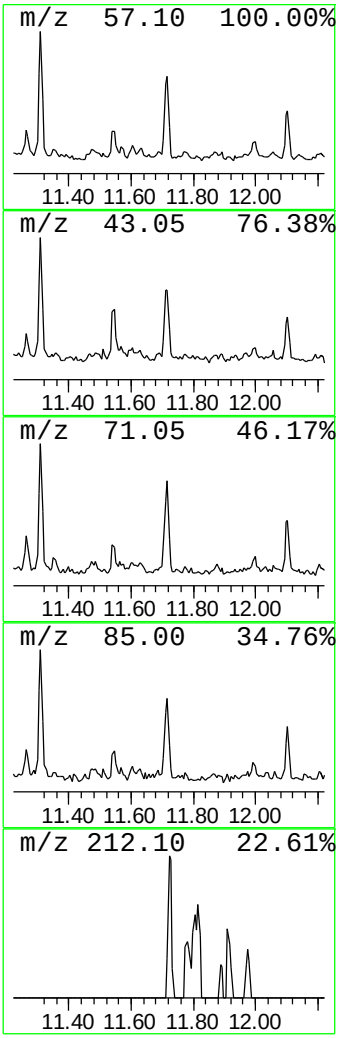
Peak Number 13 Pentadecane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.72	2.30 ng	85368	Phenanthrene-d10	10.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane	212	C15H32	000629-62-9	87
2	Tetradecane, 2-methyl-	212	C15H32	001560-95-8	80
3	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	80
4	3,5-Dimethyldodecane	198	C14H30	107770-99-0	78
5	Hexadecane	226	C16H34	000544-76-3	72





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Sample : I4397-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P-1A-4.0-4.5-072117

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
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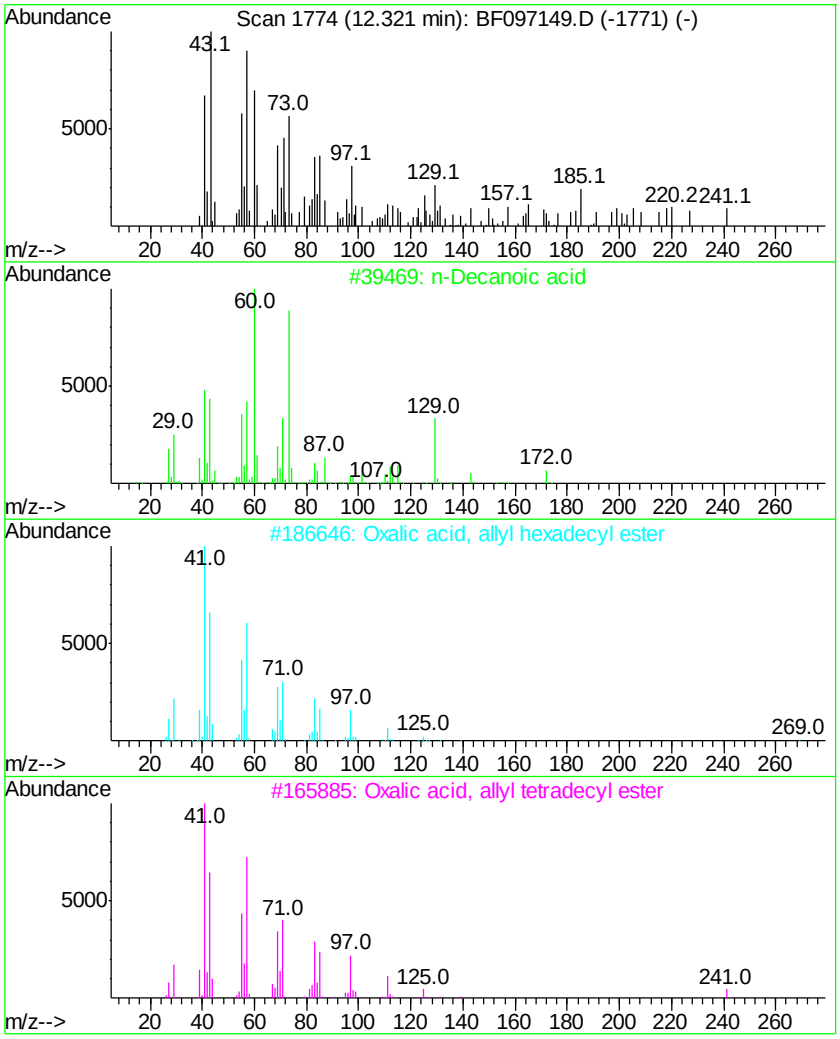
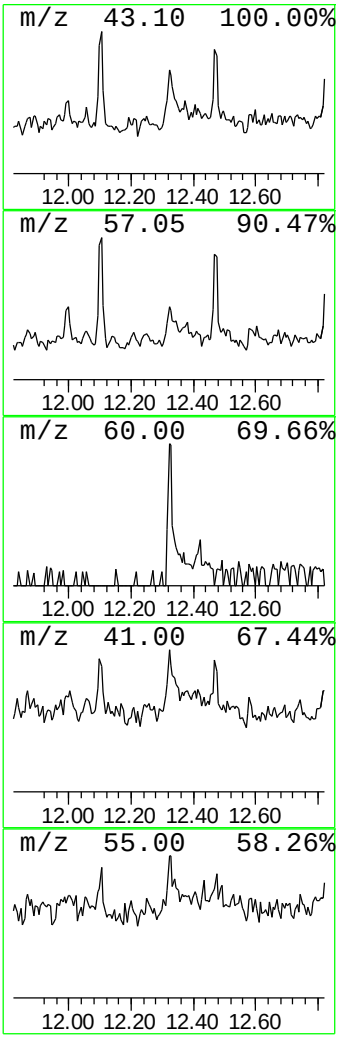
Peak Number 14 unknown12.32 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.32	2.94 ng	100192	Chrysene-d12	13.61

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Decanoic acid	172	C10H20O2	000334-48-5	41
2	Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	30
3	Oxalic acid, allyl tetradecyl ester	326	C19H34O4	1000309-24-2	30
4	Oxalic acid, cyclobutyl tetradec...	340	C20H36O4	1000309-70-9	25
5	Oxalic acid, propyl tetradecyl e...	328	C19H36O4	1000309-26-7	25





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Operator : SJ/JU
Sample : I4397-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P-1A-4.0-4.5-072117

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

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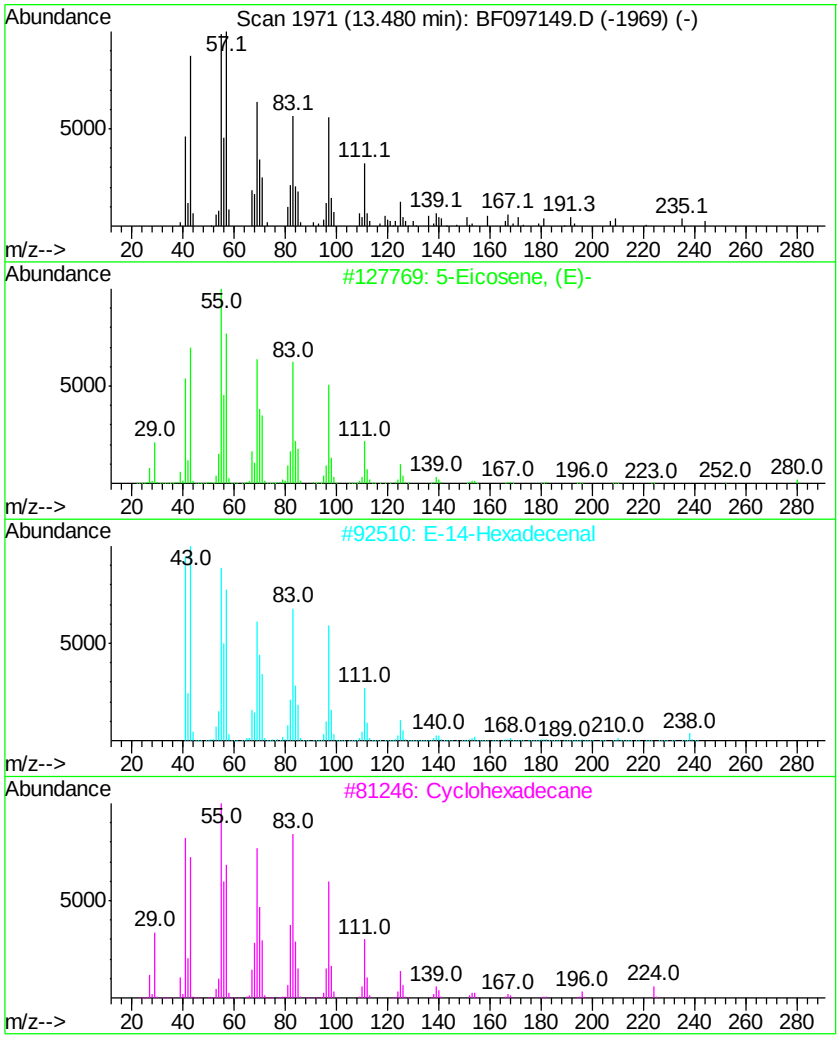
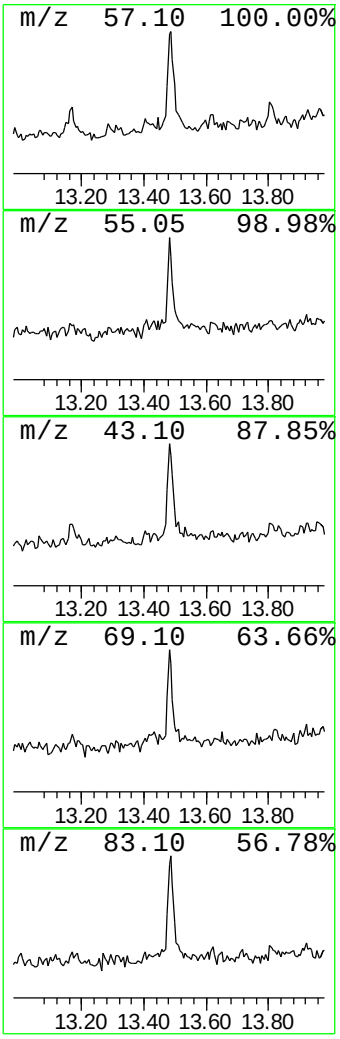
Peak Number 15 5-Eicosene, (E)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.48	4.53 ng	154578	Chrysene-d12	13.61

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	91
2	E-14-Hexadecenal	238	C16H30O	330207-53-9	90
3	Cyclohexadecane	224	C16H32	000295-65-8	81
4	Octacosanol	410	C28H58O	000557-61-9	74
5	3-Chloropropionic acid, pentadec...	318	C18H35ClO2	1000281-77-6	74





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.63	8.5	ng	296816	1	6.49	699462	20.0
unknown6.26	6.26	73.0	ng	2552030	1	6.49	699462	20.0
Hexadecane	9.97	3.3	ng	156639	3	9.52	962942	20.0
Tridecane, 6-methyl-	10.19	2.6	ng	123386	3	9.52	962942	20.0
Tridecane	10.89	3.4	ng	125123	4	10.99	743858	20.0
Hexadecane, 2,6,1...	10.92	3.1	ng	117079	4	10.99	743858	20.0
Tridecane, 2-methyl-	11.31	3.0	ng	110164	4	10.99	743858	20.0
Pentadecanoic acid	11.55	2.0	ng	75643	4	10.99	743858	20.0
unknown11.60	11.60	2.4	ng	89257	4	10.99	743858	20.0
Pentadecane	11.72	2.3	ng	85368	4	10.99	743858	20.0
unknown12.32	12.32	2.9	ng	100192	5	13.61	682039	20.0
5-Eicosene, (E)-	13.48	4.5	ng	154578	5	13.61	682039	20.0