LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092717\
Data File : BF098853.D
Acq On : 27 Sep 2017 10:33
Operator : SJ/JU
Sample : I5363-05 10X
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-3-C-COMP

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-BF092317.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	5.122	513	516	521	rBV	74339	74402	2.34%	0.407%
2	5.398	560	563	567	rBV	77153	68753	2.16%	0.376%
3	5.522	580	584	588	rBV	556887	456704	14.35%	2.496%
4	5.751	620	623	627	rVB	41690	34172	1.07%	0.187%
5	6.528	751	755	759	rBV	564541	449597	14.13%	2.457%
6	6.675	777	780	784	rBV	528699	481397	15.13%	2.631%
7	6.916	817	821	824	rVB	1007021	870238	27.35%	4.755%
8	7.069	843	847	850	rBV	469615	373721	11.74%	2.042%
9	7.469	911	915	918	rBV	355902	269400	8.47%	1.472%
10	8.198	1035	1039	1041	rBV	1205443	1141401	35.87%	6.237%
11	8.904	1156	1159	1162	rBV	44874	36083	1.13%	0.197%
12	9.269	1216	1221	1224	rBV	624389	534454	16.80%	2.920%
13	9.657	1285	1287	1291	rBV	63608	51568	1.62%	0.282%
14	9.951	1333	1337	1340	rBV	1292582	1084069	34.07%	5.924%
15	9.980	1340	1342	1345	rVB	42592	32680	1.03%	0.179%
16	10.151	1365	1371	1375	rVB3	37499	54072	1.70%	0.295%
17	10.563	1438	1441	1452	rVB2	21140	46936	1.48%	0.256%
18	10.733	1467	1470	1477	rBV	269507	222376	6.99%	1.215%
19	10.857	1486	1491	1497	rVB2	35117	51096	1.61%	0.279%
20	11.086	1524	1530	1534	rVB7	33992	46522	1.46%	0.254%
21	11.210	1548	1551	1554	rVB	37483	32404	1.02%	0.177%
22	11.321	1567	1570	1577	rVB3	17454	32793	1.03%	0.179%
23	11.439	1586	1590	1592	rBV	930241	864962	27.18%	4.726%
24	11.457	1592	1593	1597	rVV	135300	98565	3.10%	0.539%
25	11.510	1600	1602	1606	rBV	48690	43476	1.37%	0.238%
26	11.874	1660	1664	1669	rBV7	16830	33159	1.04%	0.181%
27	11.951	1672	1677	1685	rVV2	203721	264420	8.31%	1.445%
28	12.651	1792	1796	1800	rBV	174466	172738	5.43%	0.944%
29	12.739	1808	1811	1815	rBV2	63693	69862	2.20%	0.382%
30	12.863	1820	1832	1847	rBV2	1088842	3182046	100.00%	17.388%
31	13.015	1855	1858	1861	rBV	435421	413312	12.99%	2.258%
32	13.121	1868	1876	1884	rVB	1462362	3053380	95.96%	16.685%
33	13.710	1974	1976	1985	rVB3	58128	81134	2.55%	0.443%
34	13.880	2002	2005	2007	rBV	54637	54569	1.71%	0.298%

LSC Area Percent Report

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Operator : SJ/JU
Sample : I5363-05 10X
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-3-C-COMP

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-BF092317.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.074	2034	2038	2041	rBV	852521	825430	25.94%	4.510%
36	14.098	2041	2042	2048	rVB	125689	117831	3.70%	0.644%
37	14.204	2058	2060	2063	rBV	103141	92104	2.89%	0.503%
38	14.245	2064	2067	2069	rVV	147324	104265	3.28%	0.570%
39	14.274	2069	2072	2074	rBV2	60320	54498	1.71%	0.298%
40	14.362	2085	2087	2091	rBV4	43825	44489	1.40%	0.243%
41	14.586	2123	2125	2127	rBV3	43042	42030	1.32%	0.230%
42	14.921	2180	2182	2188	rVB	83047	82375	2.59%	0.450%
43	15.121	2213	2216	2219	rBV	109726	144050	4.53%	0.787%
44	15.174	2220	2225	2231	rVB5	211831	447722	14.07%	2.446%
45	15.439	2267	2270	2276	rVB	94682	125272	3.94%	0.685%
46	15.498	2277	2280	2286	rVV	77427	113665	3.57%	0.621%
47	15.568	2287	2292	2301	rVB	669172	893589	28.08%	4.883%
48	16.203	2397	2400	2407	rVB3	85278	152640	4.80%	0.834%
49	17.115	2551	2555	2568	rVB5	120163	284128	8.93%	1.553%

Sum of corrected areas: 18300549

LSC Report - Integrated Chromatogram

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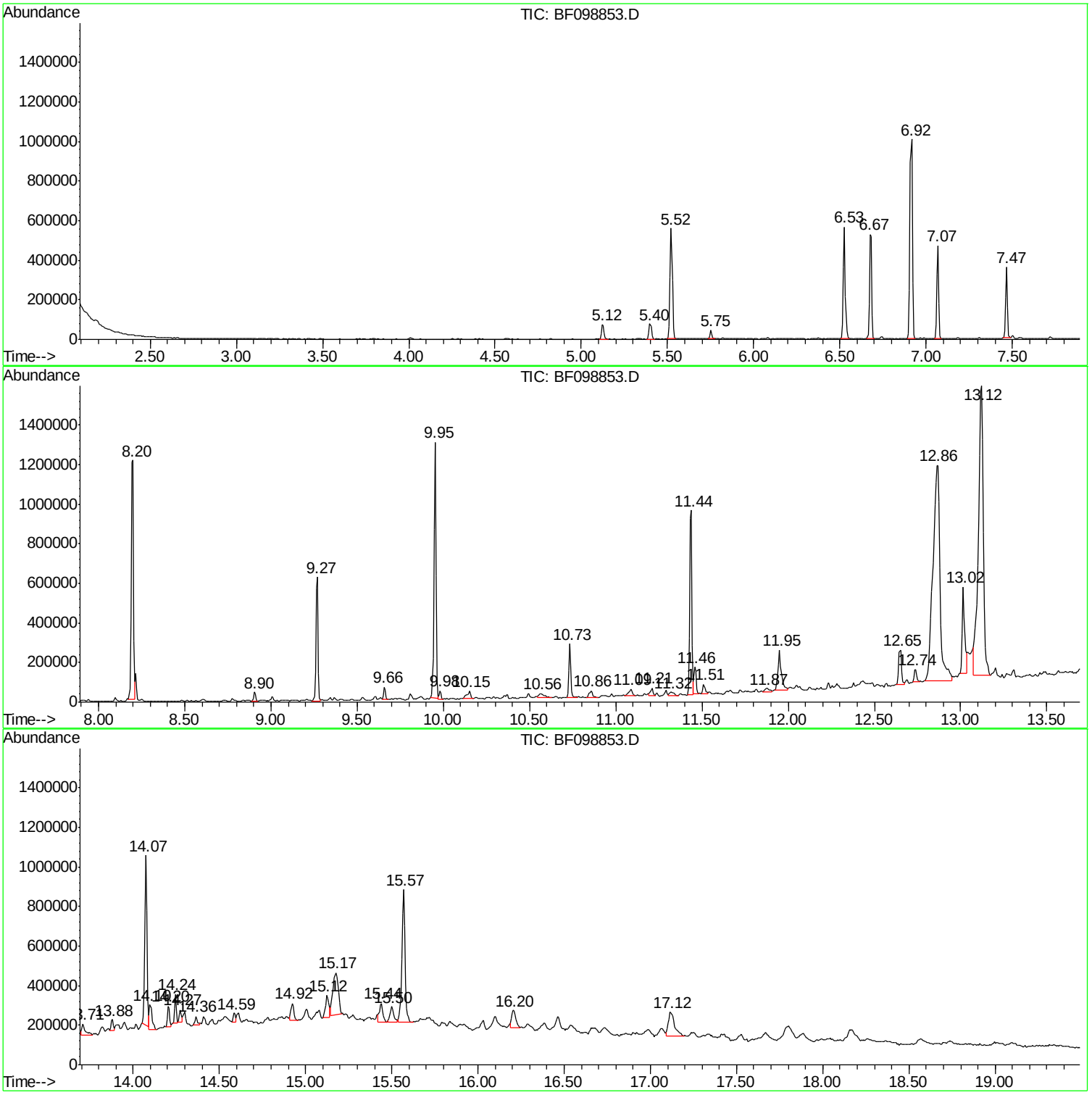
Data File : BF098853.D
Acq On : 27 Sep 2017 10:33
Operator : SJ/JU
Sample : I5363-05 10X
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-3-C-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF092717\
Data File : BF098853.D
Acq On : 27 Sep 2017 10:33
Operator : SJ/JU
Sample : I5363-05 10X
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-3-C-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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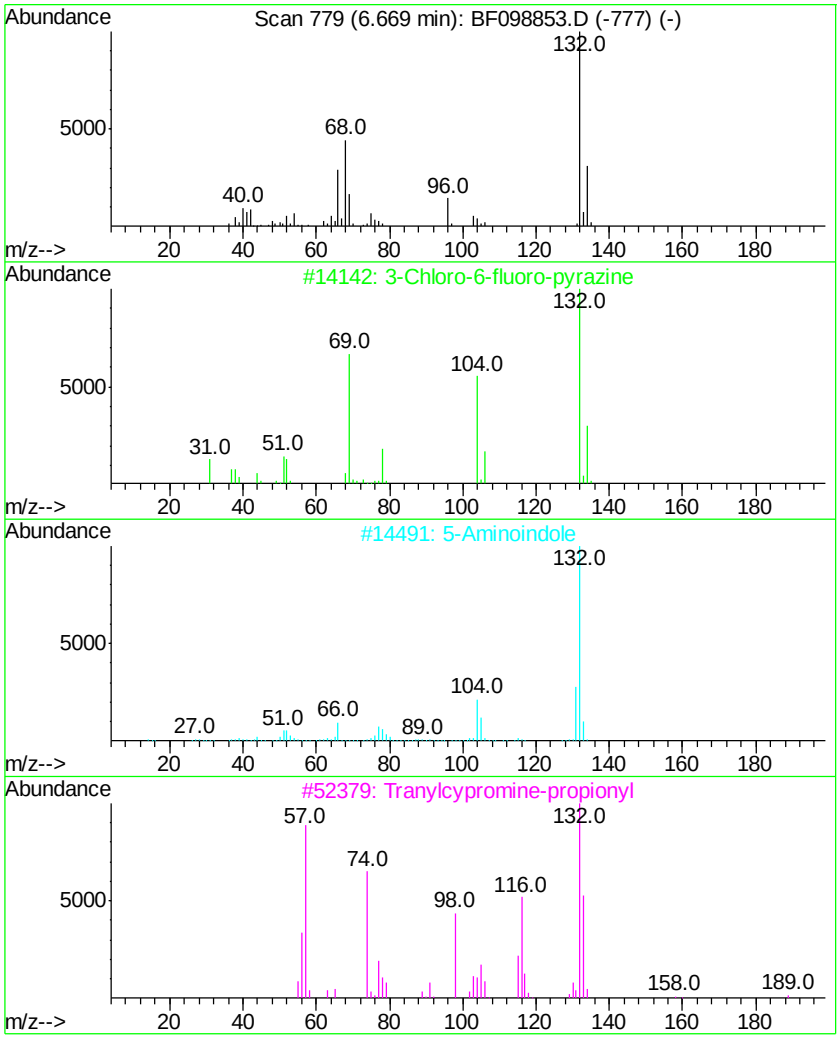
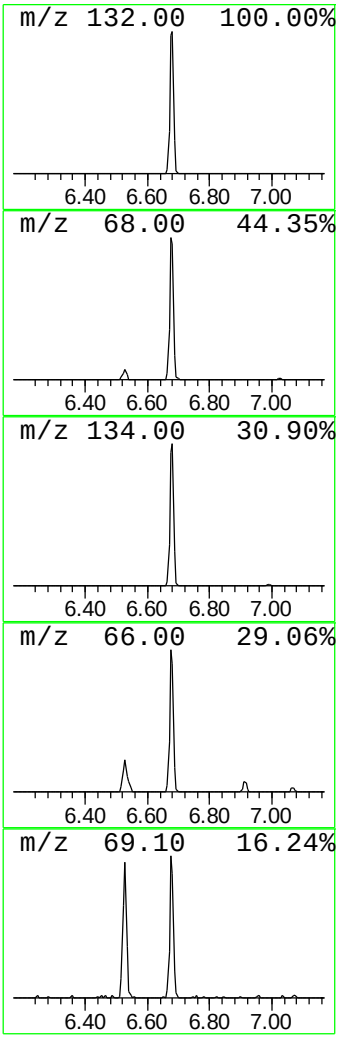
Peak Number 1 unknown6.67 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.67	11.06 ng	481397	1,4-Dichlorobenzene-d4	6.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092717\
Data File : BF098853.D
Acq On : 27 Sep 2017 10:33
Operator : SJ/JU
Sample : I5363-05 10X
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-3-C-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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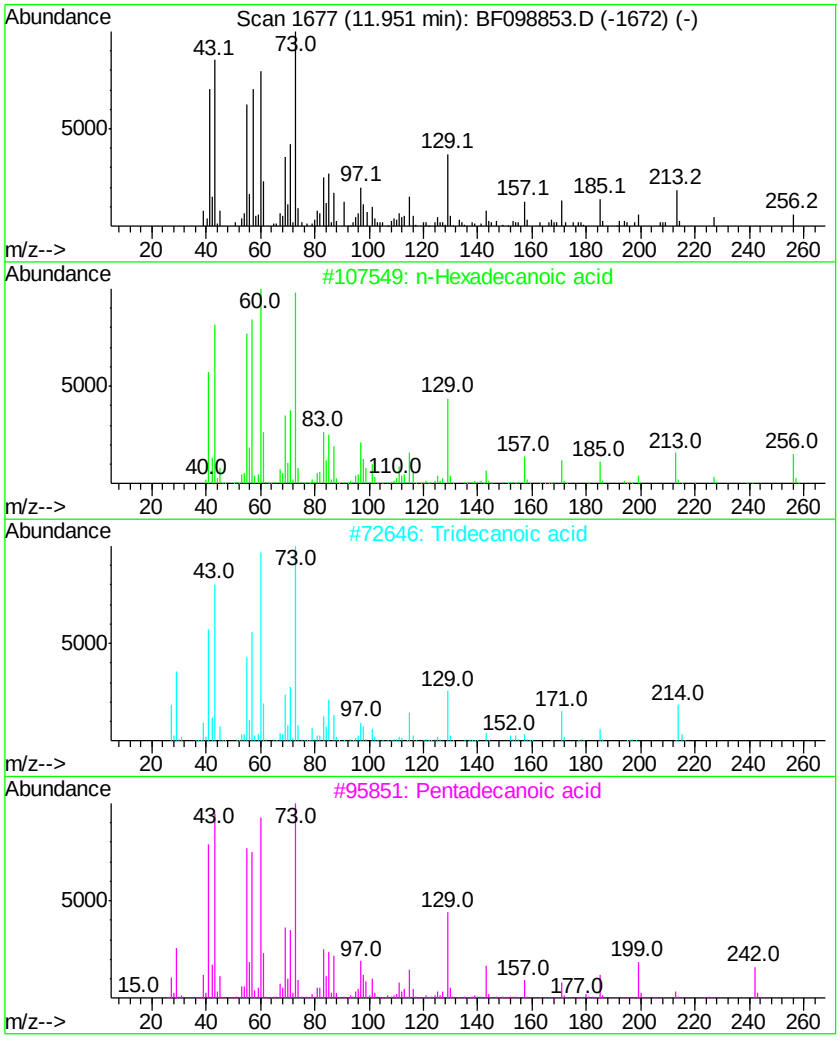
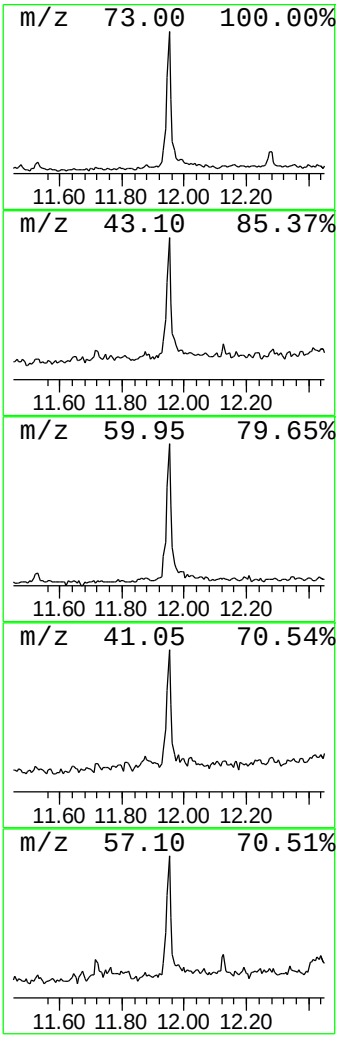
Peak Number 3 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.95	6.11 ng	264420	Phenanthrene-d10	11.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	n-Decanoic acid	172	C10H20O2	000334-48-5	62





Data Path : Z:\HPCHEM1\BNA F\DATA\BF092717\
Data File : BF098853.D
Acq On : 27 Sep 2017 10:33
Operator : SJ/JU
Sample : I5363-05 10X
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-3-C-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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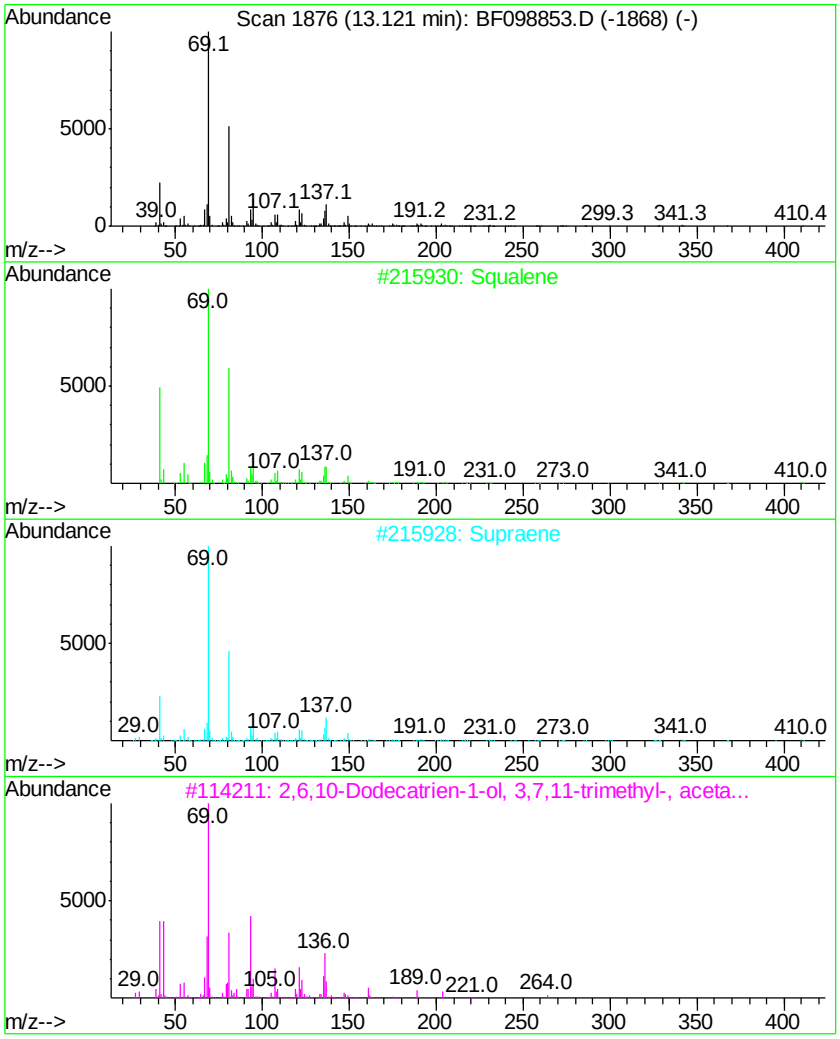
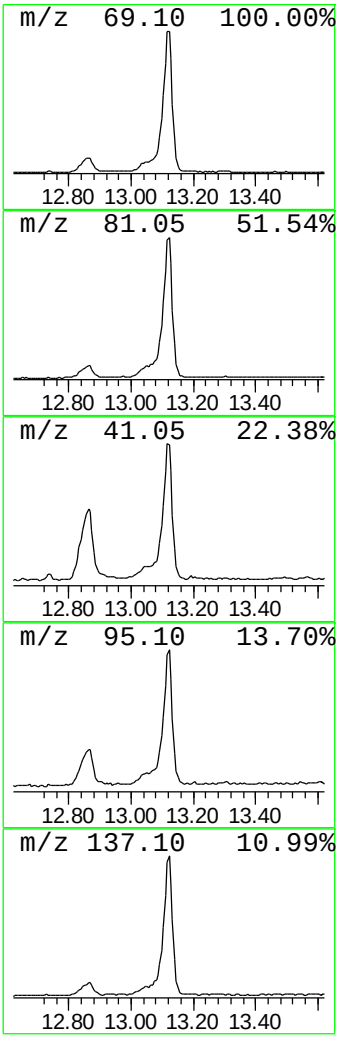
Peak Number 4 Squalene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.12	73.98 ng	3053380	Chrysene-d12	14.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	91
2	Supraene	410	C30H50	007683-64-9	91
3	2,6,10-Dodecatrien-1-ol, 3,7,11-...	264	C17H28O2	004128-17-0	64
4	2,3,5-Trimethyl-2,3,5-hexanetric...	203	C12H17N3	003974-79-6	50
5	1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	50





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ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-3-C-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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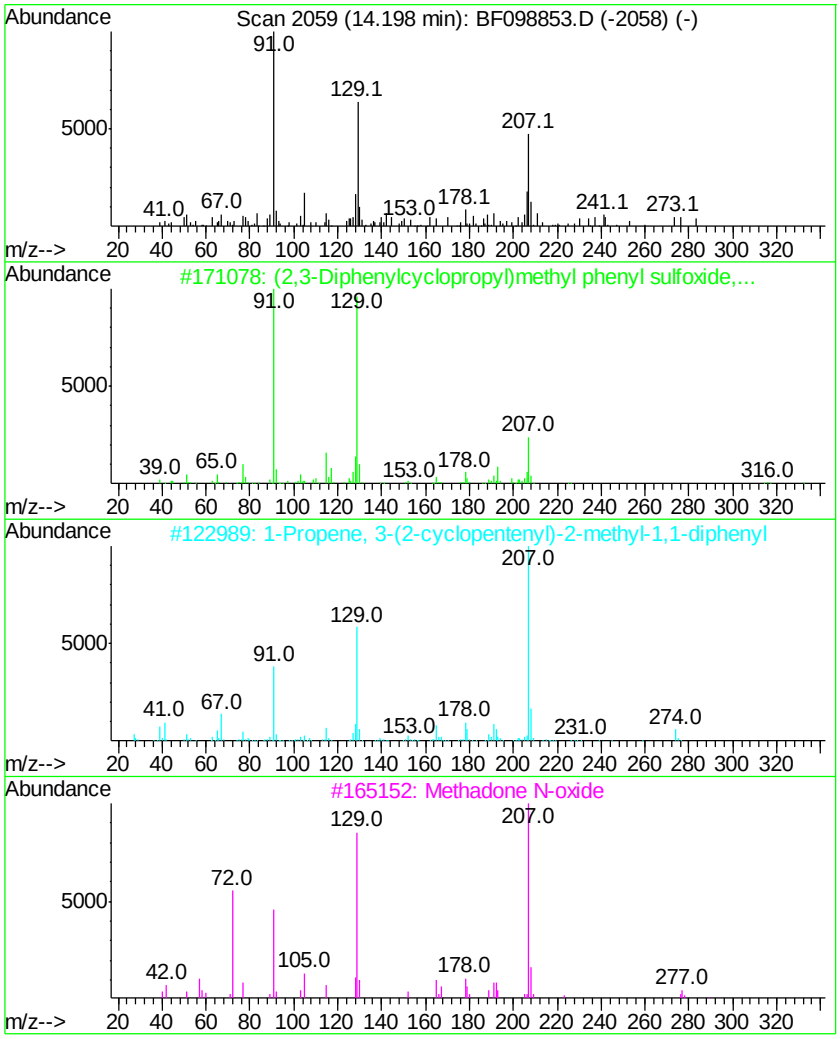
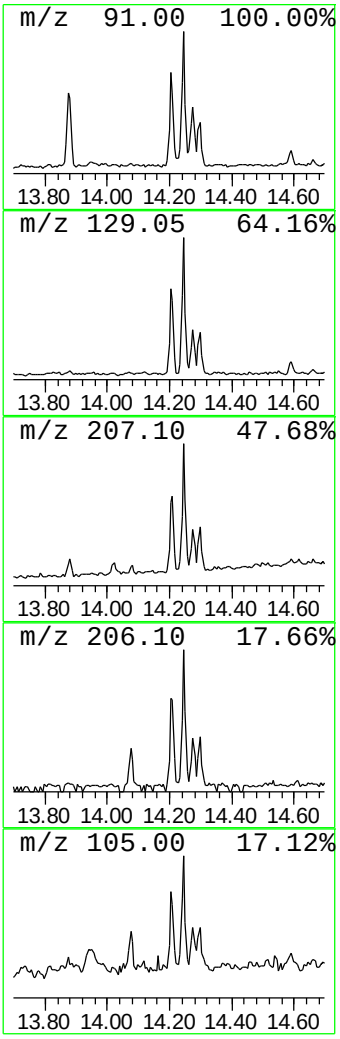
Peak Number 5 (2,3-Diphenylcyclopropyl)me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.20	2.23 ng	92104	Chrysene-d12	14.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(2,3-Diphenylcyclopropyl)methyl ...	332	C22H20OS	131758-71-9	64
2	1-Propene, 3-(2-cyclopentenyl)-2...	274	C21H22	1000154-23-3	53
3	Methadone N-oxide	325	C21H27NO2	1000120-80-7	43
4	1H-Indole, 2-methyl-3-phenyl-	207	C15H13N	004757-69-1	41
5	5-Methyl-2-phenylindolizine	207	C15H13N	036944-99-7	30





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ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-3-C-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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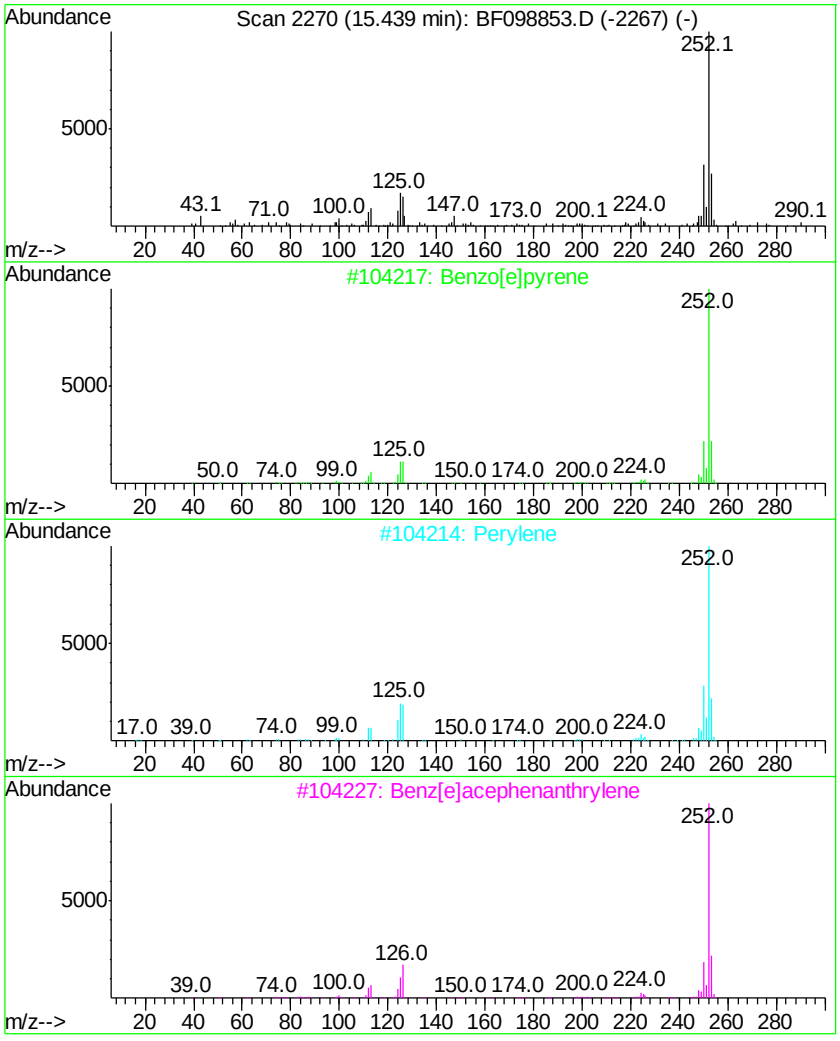
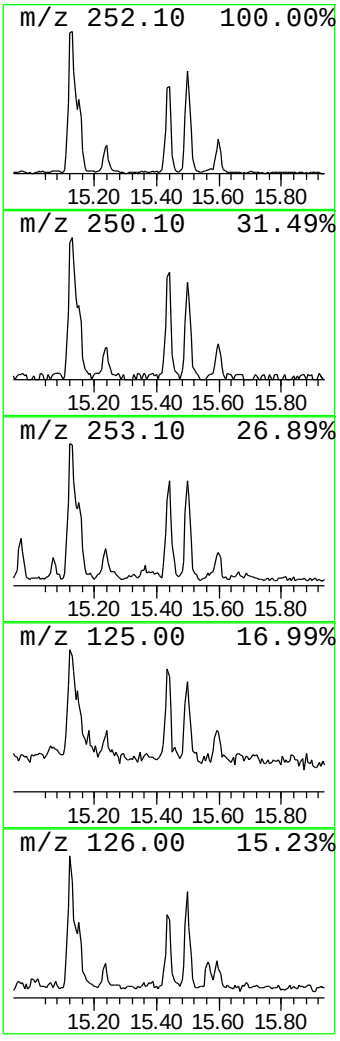
Peak Number 7 Benzo[e]pyrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.44	2.80 ng	125272	Perylene-d12	15.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2	Perylene	252	C20H12	000198-55-0	97
3	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	96
4	Benzo[k]fluoranthene	252	C20H12	000207-08-9	96
5	Benzo[j]fluoranthene	252	C20H12	000205-82-3	96





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Sample : I5363-05 10X
Misc :
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Instrument : BNA_F
ClientSampleId : SP-3-C-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

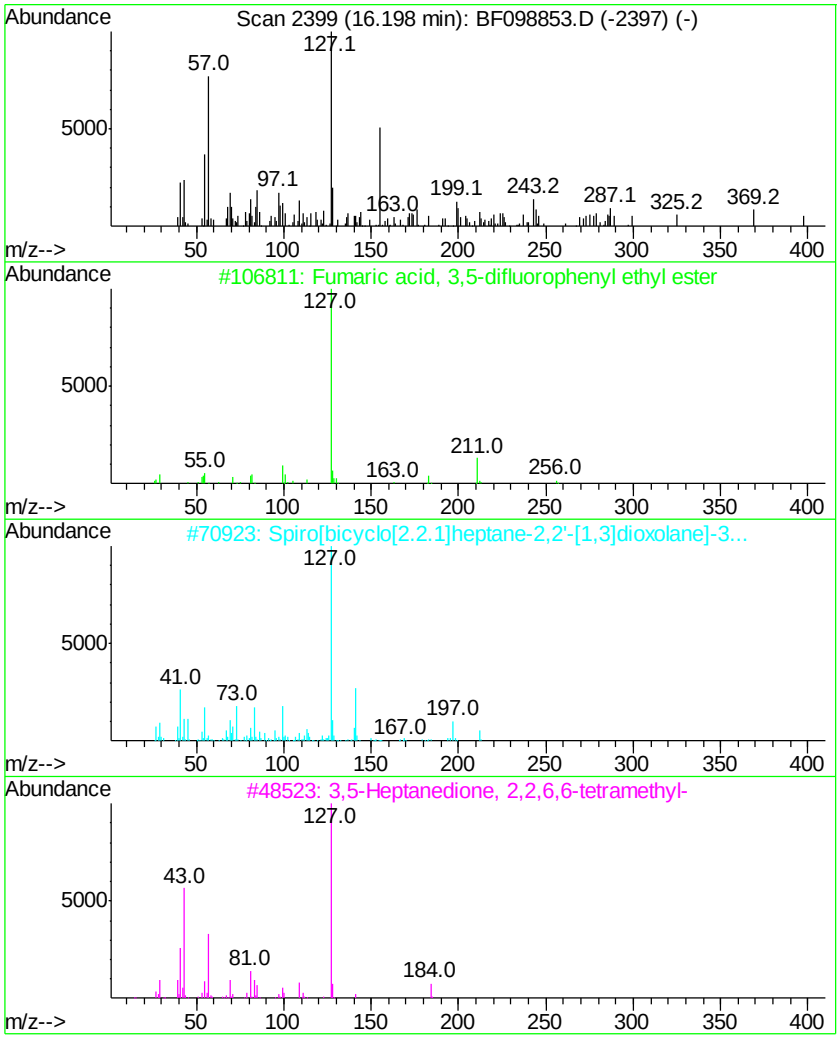
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

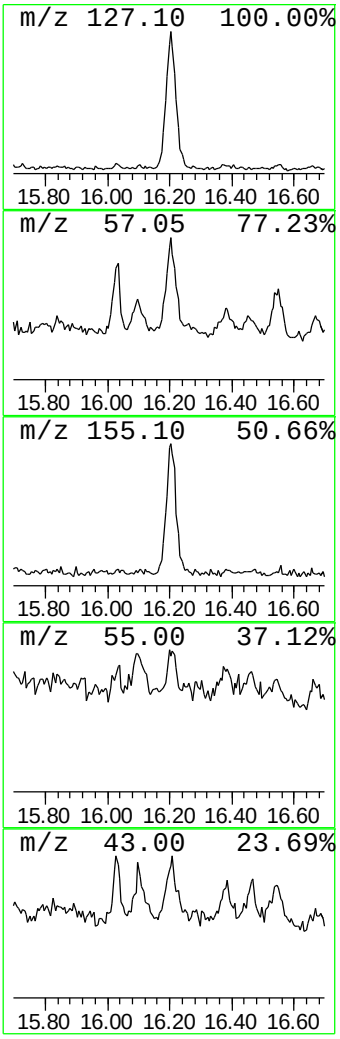
****

Peak Number 8 unknown16.20 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.20	3.42 ng	152640	Perylene-d12	15.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Fumaric acid, 3,5-difluorophenyl...	256	C12H10F2O4	1000339-36-7	35
2	Spiro[bicyclo[2.2.1]heptane-2,2'...	212	C12H20O3	035972-92-0	35
3	3,5-Heptanedione, 2,2,6,6-tetram...	184	C11H20O2	001118-71-4	35
4	Glutaric acid, 2,5-difluorobenzy...	300	C15H18F2O4	1000376-94-3	35
5	Hexanoic acid, 2-ethyl-, anhydride	270	C16H30O3	036765-89-6	35





Library Search Compound Report

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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

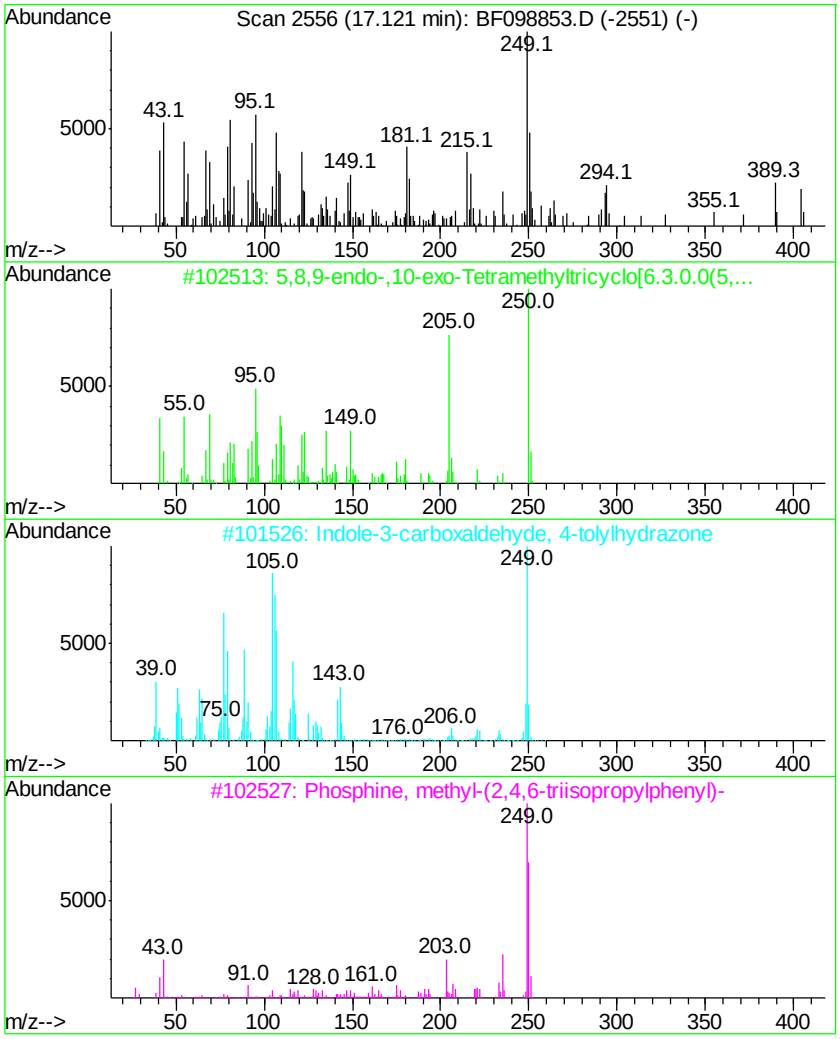
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

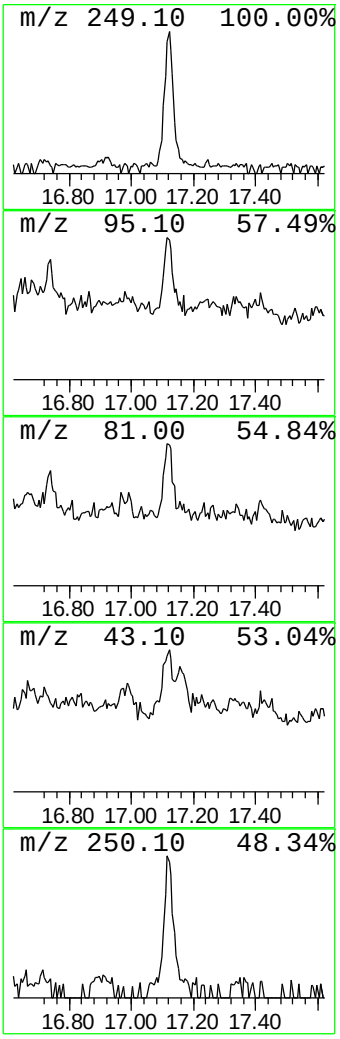
****

Peak Number 9 unknown17.12 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.12	6.36 ng	284128	Perylene-d12	15.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5,8,9-endo-,10-exo-Tetramethyltr...	250	C16H26O2	137235-57-5	25
2	Indole-3-carboxaldehyde, 4-tolyl...	249	C16H15N3	1000262-65-3	22
3	Phosphine, methyl-(2,4,6-triisop...	250	C16H27P	158748-69-7	22
4	2,6-Di-t-butyl-4-dimethylaminoph...	249	C16H27NO	010437-44-2	22
5	Cholestane-3,6-diol, (3.beta.,5....	404	C27H48O2	041083-77-6	15





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092717\
Data File : BF098853.D
Acq On : 27 Sep 2017 10:33
Operator : SJ/JU
Sample : I5363-05 10X
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-3-C-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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
unknown6.67	6.67	11.1	ng	481397	1	6.92	870238	20.0
n-Hexadecanoic acid	11.95	6.1	ng	264420	4	11.44	864962	20.0
Squalene	13.12	74.0	ng	3053380	5	14.07	825430	20.0
(2,3-Diphenylcycl...	14.20	2.2	ng	92104	5	14.07	825430	20.0
Benzo[e]pyrene	15.44	2.8	ng	125272	6	15.57	893589	20.0
unknown16.20	16.20	3.4	ng	152640	6	15.57	893589	20.0
unknown17.12	17.12	6.4	ng	284128	6	15.57	893589	20.0