LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF080317\
Data File : BF097335.D
Acq On : 3 Aug 2017 23:52
Operator : SJ/JU
Sample : I4562-22
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : JC-02-080117-H

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	4.569	453	456	475	rVB	150773	253431	10.31%	1.184%
2	5.040	532	536	556	rBV	2020266	2457399	100.00%	11.481%
3	6.116	715	719	733	rBV	2357486	2453519	99.84%	11.463%
4	6.222	733	737	744	rVB	2268027	2307042	93.88%	10.778%
5	6.445	772	775	783	rVB	850665	775517	31.56%	3.623%
6	6.598	797	801	810	rBV	1824338	1711775	69.66%	7.997%
7	7.016	868	872	879	rBV	1657547	1477118	60.11%	6.901%
8	7.163	895	897	903	rVB4	22384	30238	1.23%	0.141%
9	7.251	909	912	918	rVB4	45950	42179	1.72%	0.197%
10	7.369	925	932	936	rBV5	51970	63826	2.60%	0.298%
11	7.728	989	993	1005	rVB	1109764	997723	40.60%	4.661%
12	7.939	1026	1029	1033	rVB4	26476	26430	1.08%	0.123%
13	8.175	1064	1069	1076	rBV3	48784	79724	3.24%	0.372%
14	8.339	1093	1097	1101	rBV4	20719	35181	1.43%	0.164%
15	8.439	1111	1114	1117	rVB2	28556	27997	1.14%	0.131%
16	8.675	1151	1154	1158	rBV7	17354	25677	1.04%	0.120%
17	8.804	1171	1176	1179	rBV	2293958	2077816	84.55%	9.707%
18	9.069	1217	1221	1225	rBV2	29432	44918	1.83%	0.210%
19	9.133	1229	1232	1234	rBV	30731	34970	1.42%	0.163%
20	9.198	1241	1243	1249	rBV	290187	263537	10.72%	1.231%
21	9.328	1262	1265	1268	rBV	29816	29831	1.21%	0.139%
22	9.380	1271	1274	1278	rVB5	26651	27654	1.13%	0.129%
23	9.428	1278	1282	1284	rBV	43492	41974	1.71%	0.196%
24	9.469	1284	1289	1292	rBV	814863	764948	31.13%	3.574%
25	9.580	1304	1308	1312	rVB3	19673	31809	1.29%	0.149%
26	9.675	1318	1324	1328	rBV4	28508	49574	2.02%	0.232%
27	9.745	1334	1336	1340	rVB3	34980	30874	1.26%	0.144%
28	9.786	1340	1343	1347	rBV5	28188	43420	1.77%	0.203%
29	9.869	1354	1357	1360	rBV4	29103	36211	1.47%	0.169%
30	9.922	1363	1366	1370	rVB	66729	56519	2.30%	0.264%
31	10.139	1399	1403	1406	rBV	59445	71436	2.91%	0.334%
32	10.251	1419	1422	1428	rBV	1007317	931190	37.89%	4.350%
33	10.404	1442	1448	1453	rVB	118402	180170	7.33%	0.842%
34	10.580	1476	1478	1482	rBV4	34309	39211	1.60%	0.183%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF080317\
Data File : BF097335.D
Acq On : 3 Aug 2017 23:52
Operator : SJ/JU
Sample : I4562-22
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : JC-02-080117-H

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	10.680	1491	1495	1496	rBV4	20003	25293	1.03%	0.118%
36	10.833	1518	1521	1524	rBV	67141	63721	2.59%	0.298%
37	10.863	1524	1526	1533	rVB	90076	101333	4.12%	0.473%
38	10.939	1535	1539	1541	rBV	672702	577946	23.52%	2.700%
39	10.963	1541	1543	1547	rVV	81405	74796	3.04%	0.349%
40	11.016	1549	1552	1556	rVB3	35109	38786	1.58%	0.181%
41	11.257	1591	1593	1598	rBV2	49366	56587	2.30%	0.264%
42	11.357	1608	1610	1615	rVB6	35333	39993	1.63%	0.187%
43	11.439	1622	1624	1627	rBV2	30794	28185	1.15%	0.132%
44	11.469	1627	1629	1631	rVB	44932	32986	1.34%	0.154%
45	11.498	1631	1634	1640	rBV2	109018	133285	5.42%	0.623%
46	11.551	1640	1643	1645	rBV2	44924	47446	1.93%	0.222%
47	11.674	1660	1664	1667	rBV2	54567	78870	3.21%	0.368%
48	11.786	1681	1683	1685	rVB2	41616	29422	1.20%	0.137%
49	11.863	1694	1696	1697	rBV	39840	28094	1.14%	0.131%
50	11.986	1715	1717	1719	rBV	61889	54164	2.20%	0.253%
51	12.145	1741	1744	1749	rBV	143638	152123	6.19%	0.711%
52	12.192	1749	1752	1757	rBV6	56683	88804	3.61%	0.415%
53	12.368	1779	1782	1785	rBV	128407	123522	5.03%	0.577%
54	12.521	1804	1808	1814	rBV	1445054	1381713	56.23%	6.455%
55	13.445	1963	1965	1970	rVB2	198774	197413	8.03%	0.922%
56	13.563	1982	1985	1988	rBV	524912	529411	21.54%	2.473%

Sum of corrected areas: 21404731

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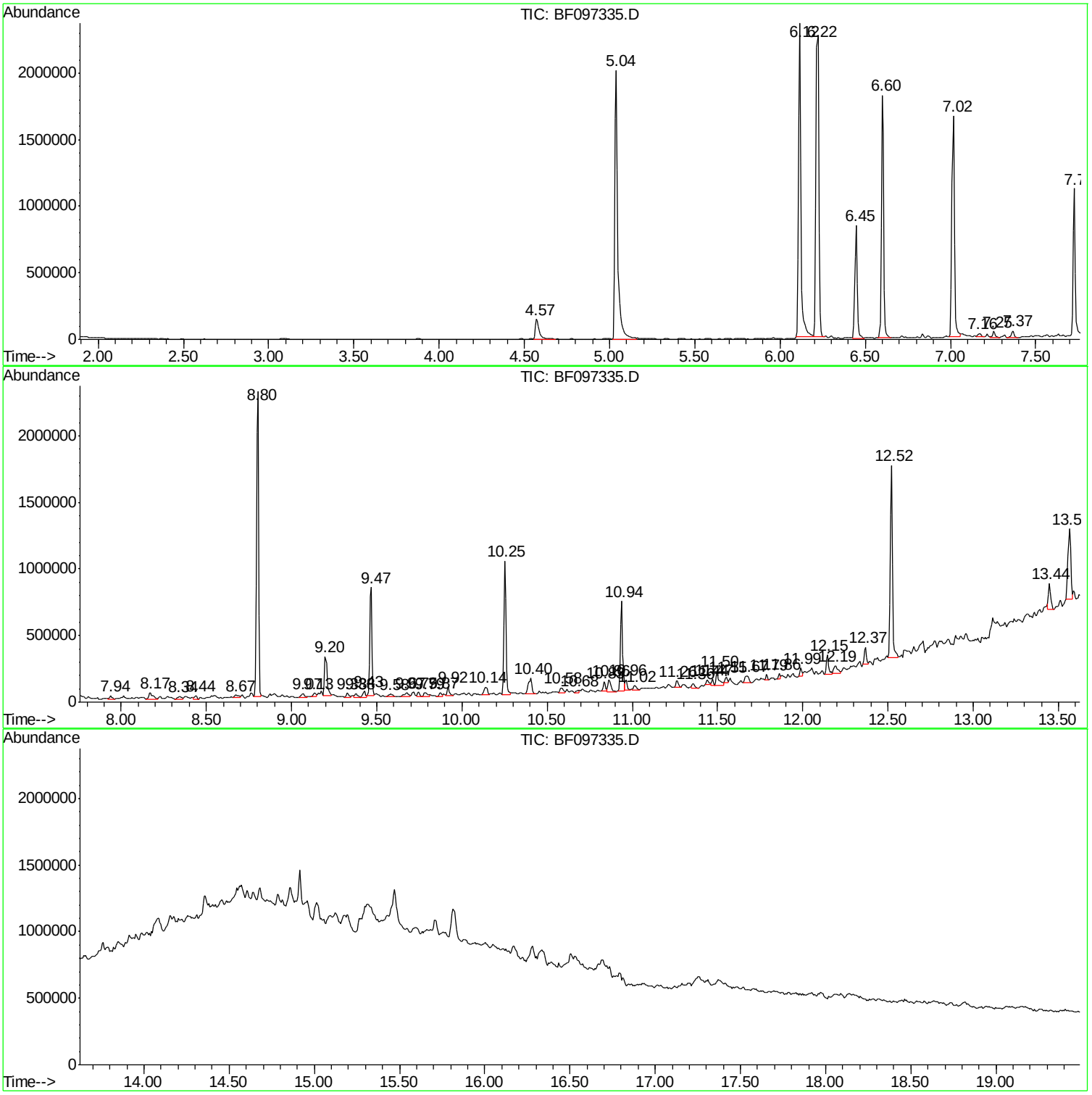
Instrument : BNA_F
ClientSampleId : JC-02-080117-H

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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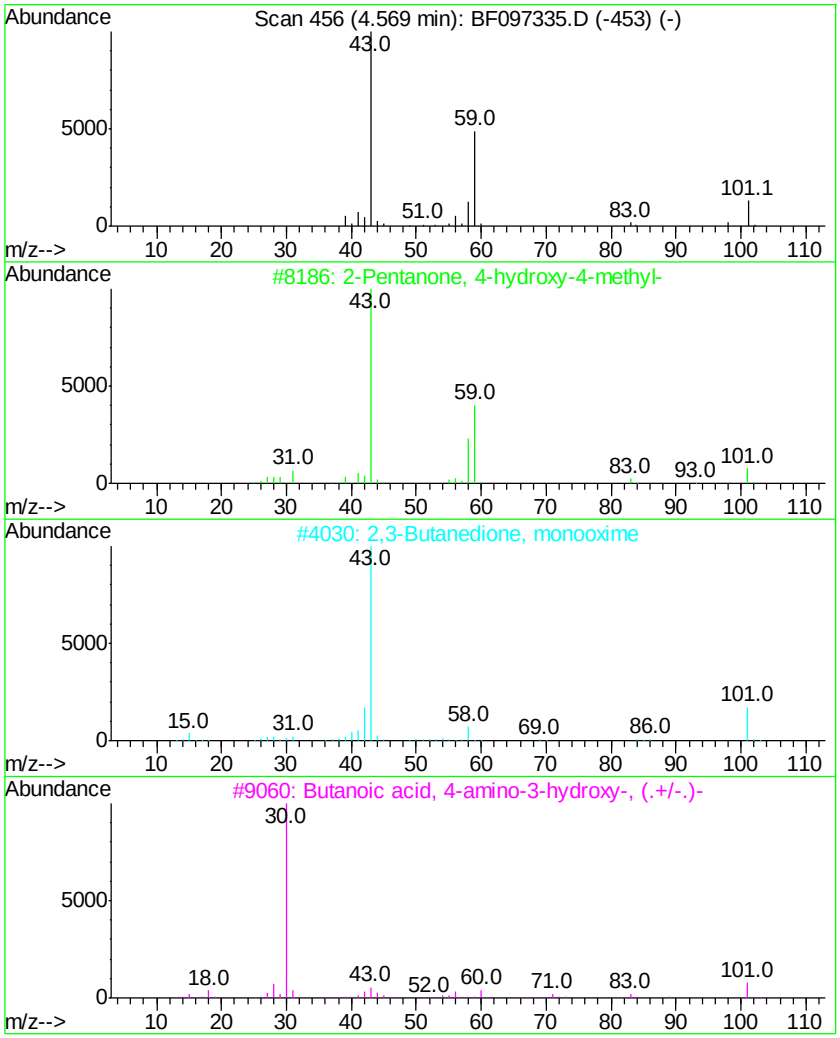
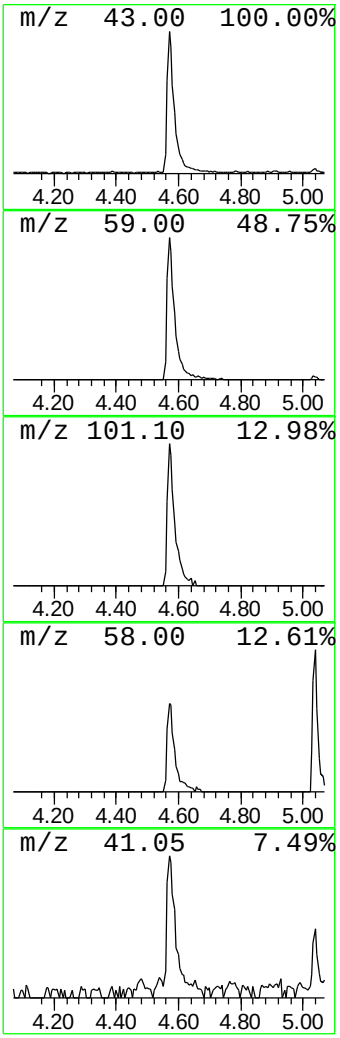
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.57	6.54 ng	253431	1,4-Dichlorobenzene-d4	6.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
3	Butanoic acid, 4-amino-3-hydroxy...	119	C4H9NO3	000924-49-2	9
4	5-Aminovaleric acid	117	C5H11NO2	000660-88-8	9
5	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9





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Sample : I4562-22
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Instrument : BNA_F
ClientSampleId : JC-02-080117-H

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

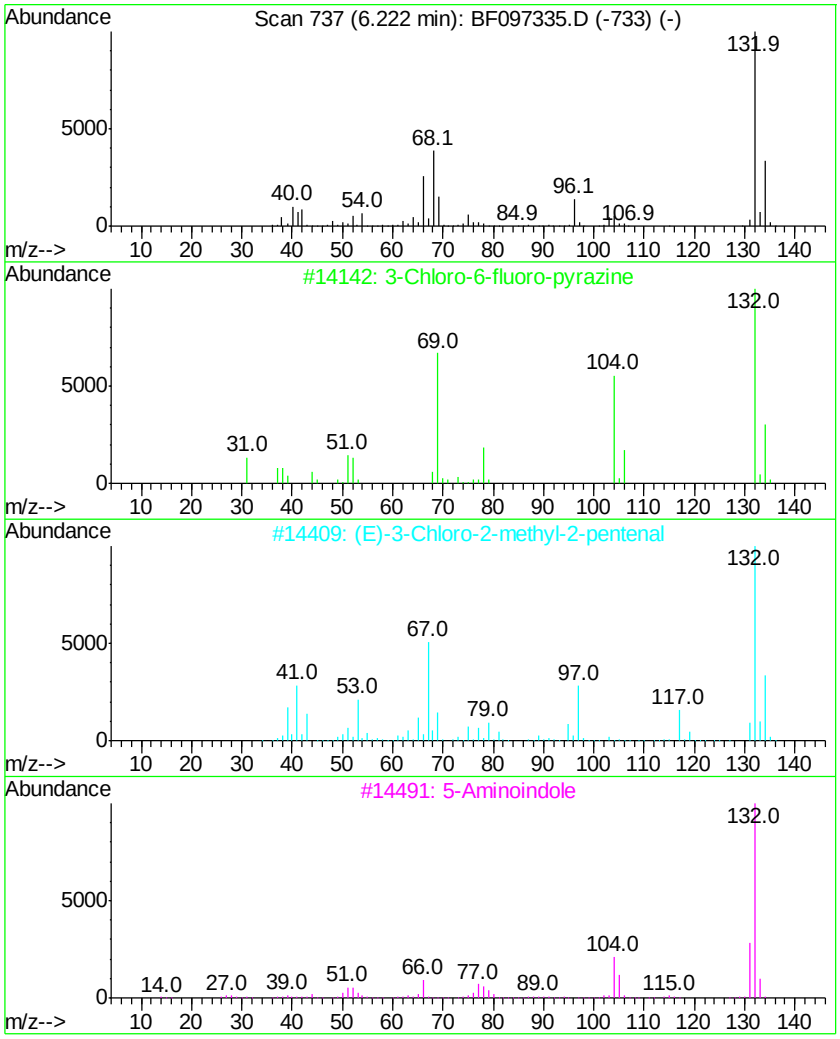
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

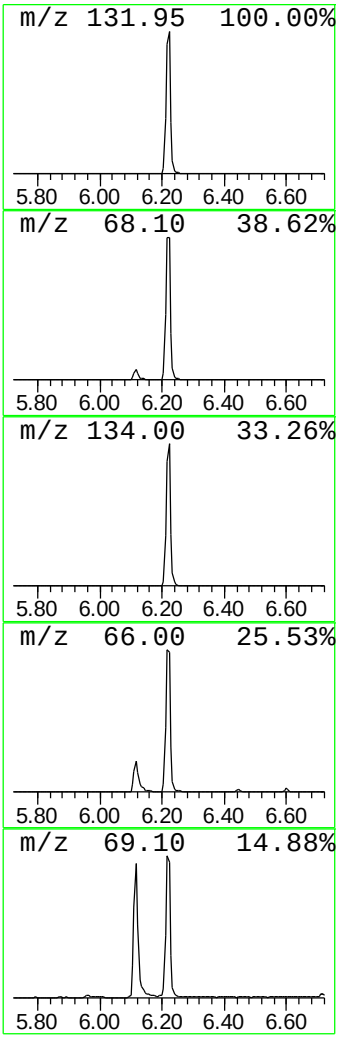
****

Peak Number 2 unknown6.22 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.22	59.50 ng	2307040	1,4-Dichlorobenzene-d4	6.45

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	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





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Instrument : BNA_F
ClientSampleId : JC-02-080117-H

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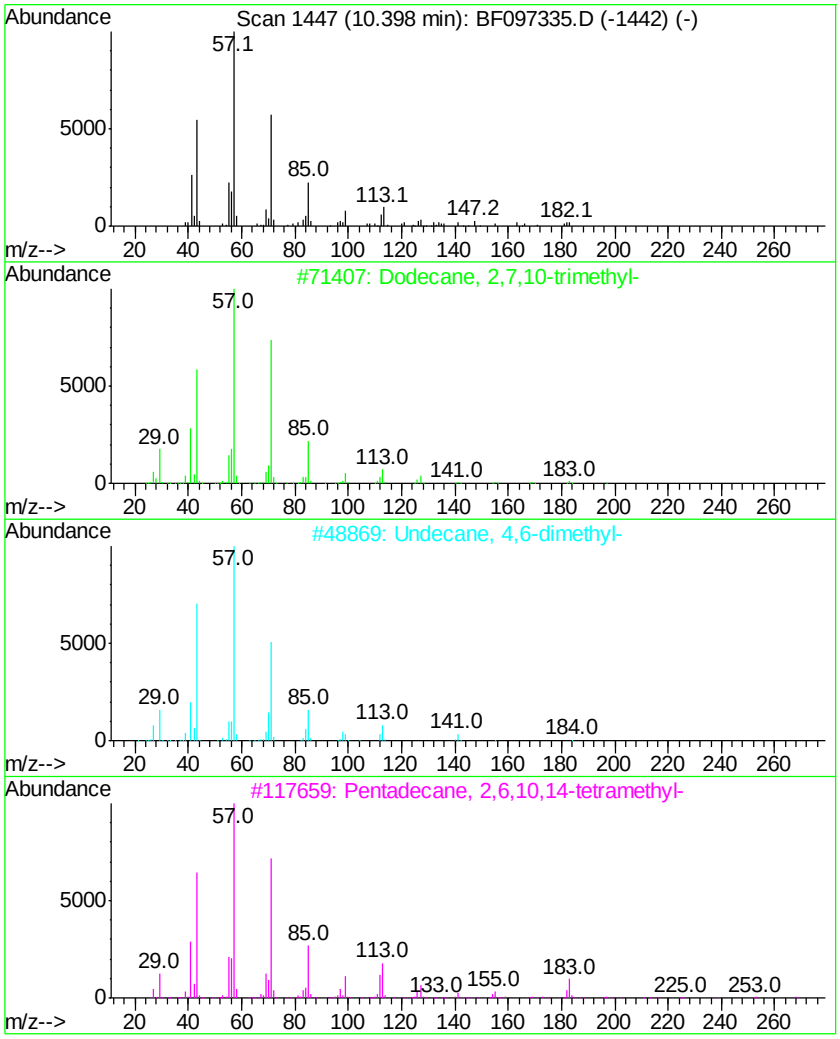
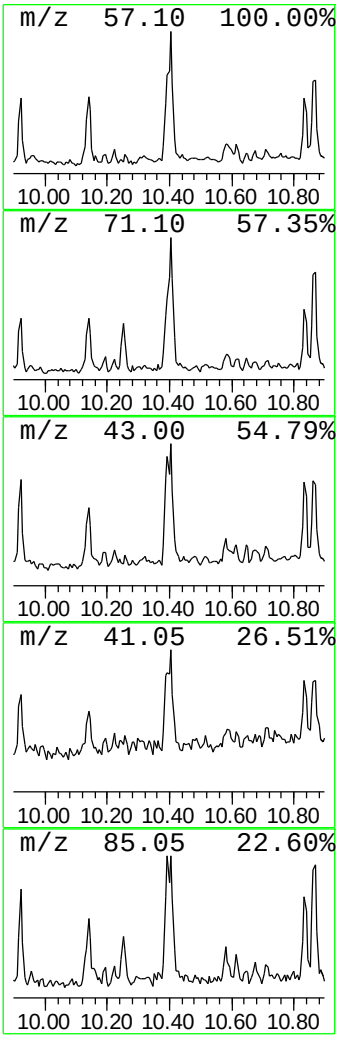
****

Peak Number 4 Dodecane, 2,7,10-trimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.40	6.23 ng	180170	Phenanthrene-d10	10.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	90
2	Undecane, 4,6-dimethyl-	184	C13H28	017312-82-2	78
3	Pentadecane, 2,6,10,14-tetramethyl-	268	C19H40	001921-70-6	78
4	Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	78
5	Decane, 2-methyl-	156	C11H24	006975-98-0	78





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Sample : I4562-22
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ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : JC-02-080117-H

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

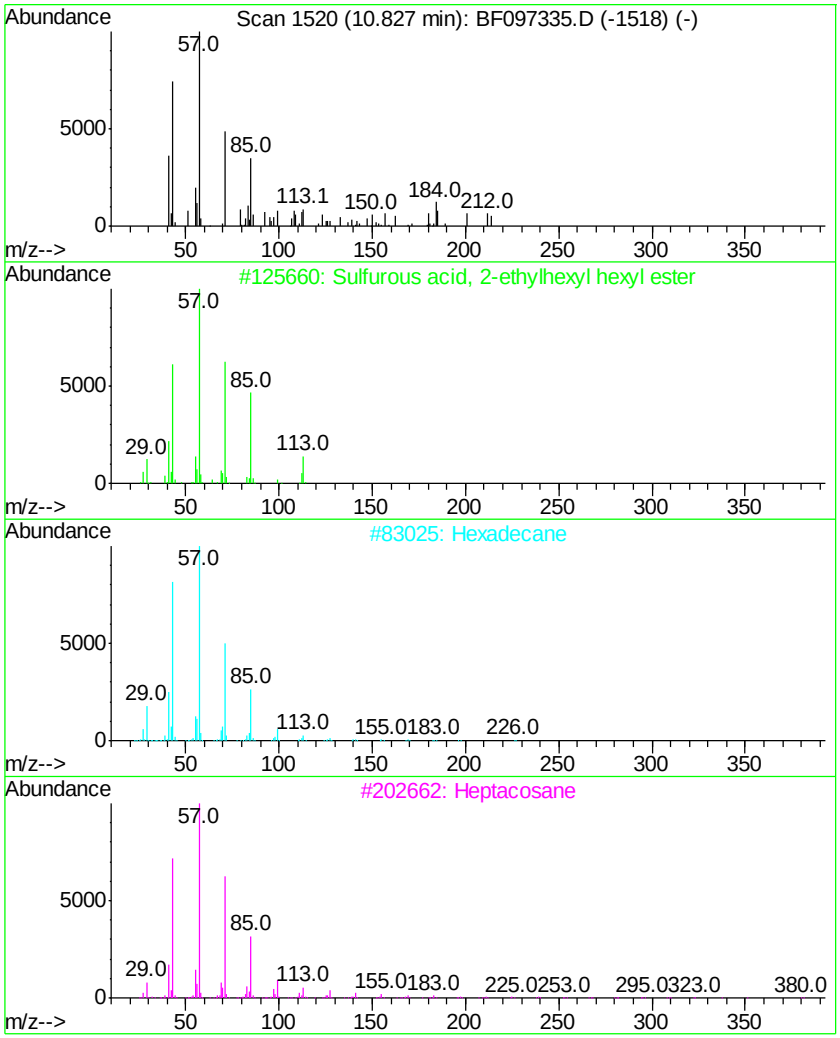
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

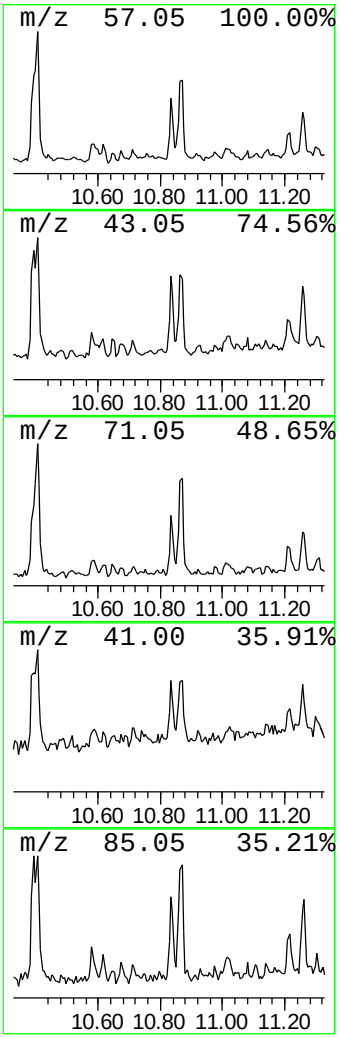
****

Peak Number 5 Sulfurous acid, 2-ethylhexy... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.83	2.21 ng	63721	Phenanthrene-d10	10.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	53
2	Hexadecane	226	C16H34	000544-76-3	52
3	Heptacosane	380	C27H56	000593-49-7	52
4	3-Methyl-4-(methoxycarbonyl)hexa...	184	C9H12O4	1000104-10-8	49
5	Hexacosane	366	C26H54	000630-01-3	49





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Instrument : BNA_F
ClientSampleId : JC-02-080117-H

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

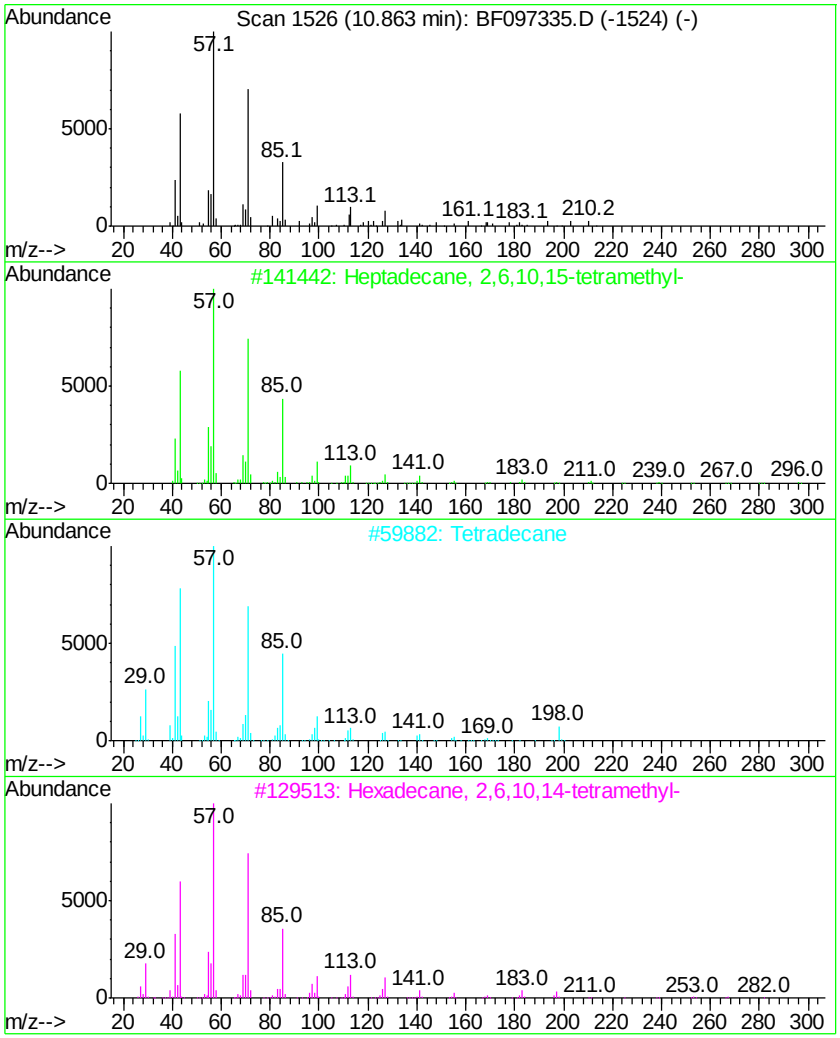
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

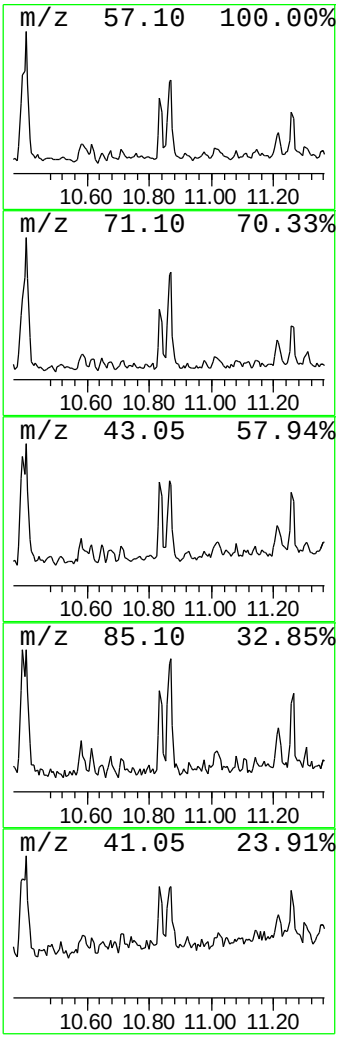
****

Peak Number 6 Heptadecane, 2,6,10,15-tetr... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.86	3.51 ng	101333	Phenanthrene-d10	10.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	86
2	Tetradecane	198	C14H30	000629-59-4	78
3	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	72
4	Disulfide, di-tert-dodecyl	402	C24H50S2	027458-90-8	64
5	Sulfurous acid, 2-ethylhexyl non...	320	C17H36O3S	1000309-19-2	58





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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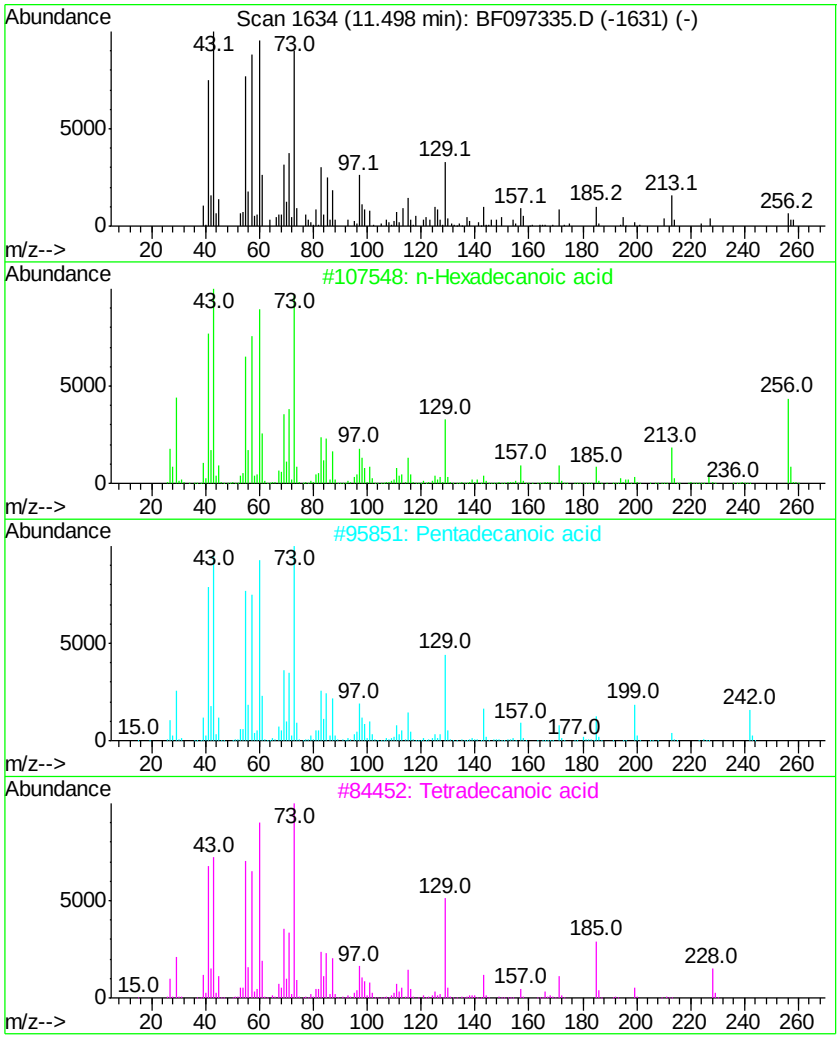
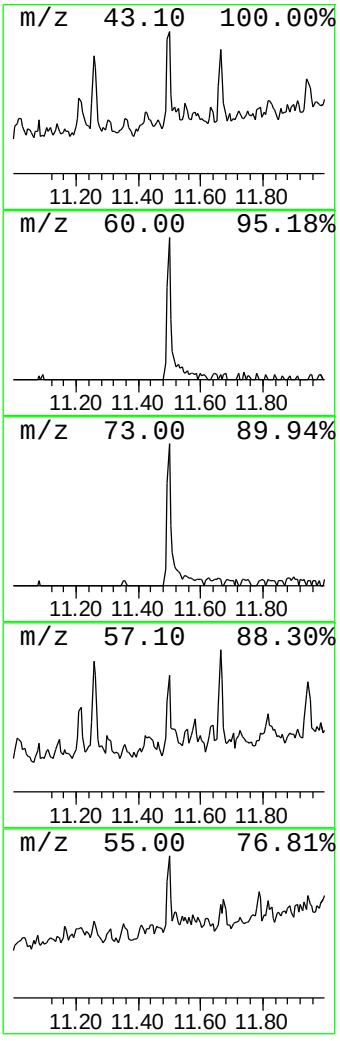
Peak Number 7 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.50	4.61 ng	133285	Phenanthrene-d10	10.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4	Dodecanoic acid	200	C12H24O2	000143-07-7	59
5	Undecanoic acid	186	C11H22O2	000112-37-8	53





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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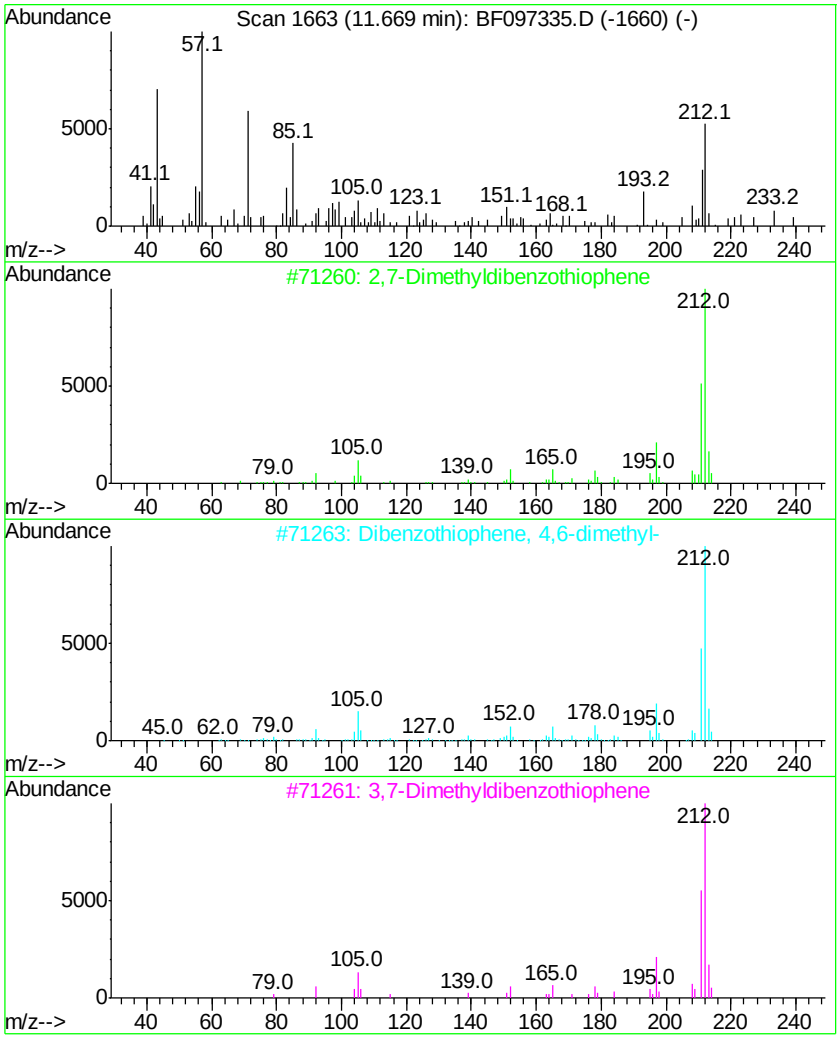
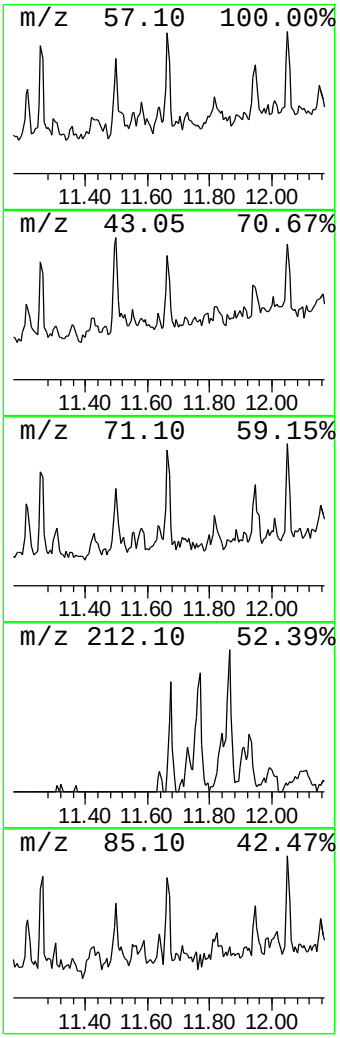
Peak Number 8 2,7-Dimethyldibenzothiophene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.67	2.73 ng	78870	Phenanthrene-d10	10.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,7-Dimethyldibenzothiophene	212	C14H12S	031317-19-8	50
2	Dibenzothiophene, 4,6-dimethyl-	212	C14H12S	001207-12-1	50
3	3,7-Dimethyldibenzothiophene	212	C14H12S	001136-85-2	50
4	1,7-Dimethyldibenzothiophene	212	C14H12S	089816-53-5	46
5	Naphtho[2,3-b]thiophene, 4,9-dim...	212	C14H12S	016587-34-1	46





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF080317\
Data File : BF097335.D
Acq On : 3 Aug 2017 23:52
Operator : SJ/JU
Sample : I4562-22
Misc :
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Instrument : BNA_F
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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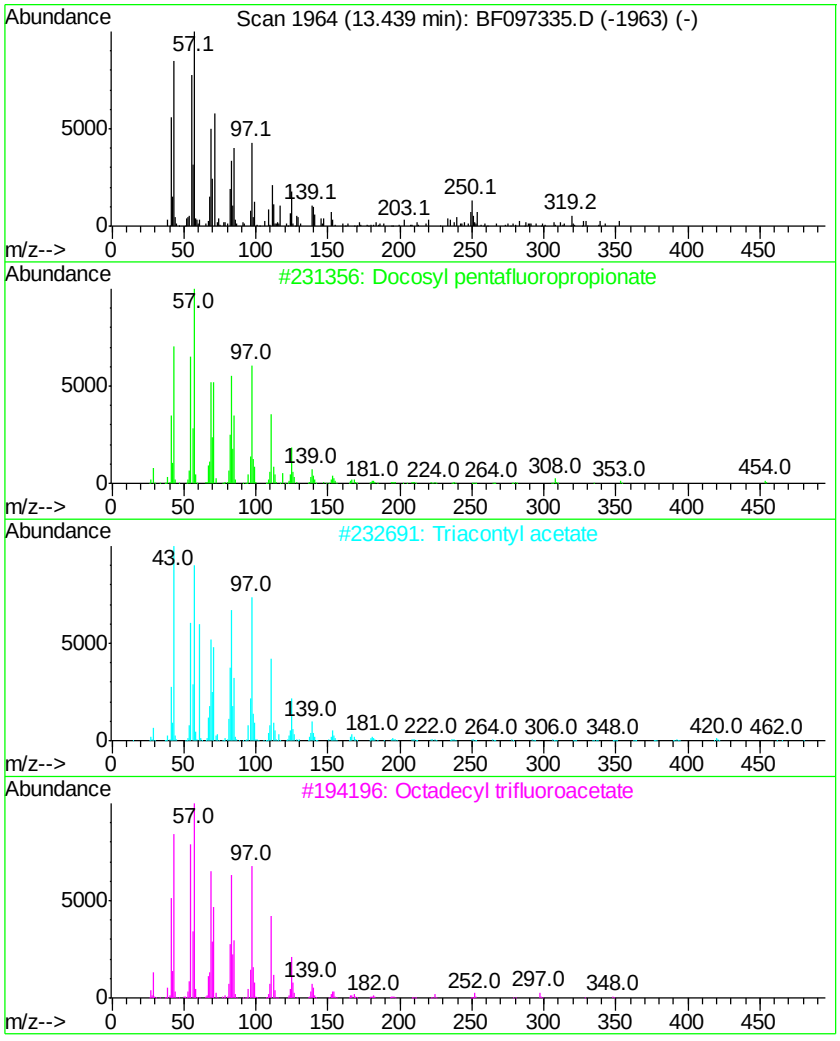
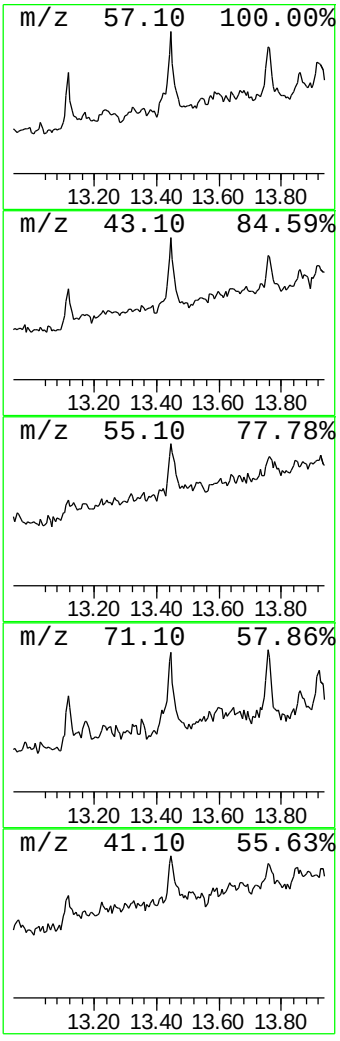
Peak Number 9 Docosyl pentafluoropropionate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.44	7.46 ng	197413	Chrysene-d12	13.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	64
2	Triacontyl acetate	480	C32H64O2	041755-58-2	58
3	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	52
4	Oxalic acid, cyclobutyl heptadec...	382	C23H42O4	1000309-70-7	46
5	Heptacosyl acetate	438	C29H58O2	1000351-78-2	46





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080317\
Data File : BF097335.D
Acq On : 3 Aug 2017 23:52
Operator : SJ/JU
Sample : I4562-22
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : JC-02-080117-H

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...	4.57	6.5	ng	253431	1	6.45	775517	20.0
unknown6.22	6.22	59.5	ng	2307040	1	6.45	775517	20.0
Dodecane, 2,7,10-...	10.40	6.2	ng	180170	4	10.94	577946	20.0
Sulfurous acid, 2...	10.83	2.2	ng	63721	4	10.94	577946	20.0
Heptadecane, 2,6,...	10.86	3.5	ng	101333	4	10.94	577946	20.0
n-Hexadecanoic acid	11.50	4.6	ng	133285	4	10.94	577946	20.0
2,7-Dimethyldiben...	11.67	2.7	ng	78870	4	10.94	577946	20.0
Docosyl pentafluo...	13.44	7.5	ng	197413	5	13.56	529411	20.0