LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF090717\
Data File : BF098330.D
Acq On : 7 Sep 2017 22:58
Operator : SJ/JU
Sample : I5071-08
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G58A-2.5-5

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-BF081517.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	4.875	471	474	484	rVB	168791	222546	8.22%	0.815%
2	5.298	541	546	549	rBV	2469673	2499549	92.37%	9.148%
3	6.339	717	723	726	rBV	2491962	2690450	99.42%	9.847%
4	6.463	739	744	747	rBV	2610135	2519379	93.10%	9.221%
5	6.516	750	753	759	rVB2	17694	29463	1.09%	0.108%
6	6.686	779	782	790	rBV	704299	629326	23.26%	2.303%
7	6.845	805	809	812	rBV	2183810	1976257	73.03%	7.233%
8	7.257	874	879	882	rBV	1660220	1587417	58.66%	5.810%
9	7.369	895	898	903	rBV	38800	41003	1.52%	0.150%
10	7.974	995	1001	1003	rBV	953416	837096	30.93%	3.064%
11	7.992	1003	1004	1007	rVB	58943	36973	1.37%	0.135%
12	8.398	1069	1073	1078	rBV	31403	32363	1.20%	0.118%
13	8.616	1106	1110	1115	rVV2	33723	42265	1.56%	0.155%
14	8.686	1119	1122	1125	rVB	55104	43492	1.61%	0.159%
15	8.786	1136	1139	1142	rBV	38376	35708	1.32%	0.131%
16	9.051	1179	1184	1187	rBV	2826302	2706145	100.00%	9.905%
17	9.133	1194	1198	1200	rBV2	36562	36232	1.34%	0.133%
18	9.386	1238	1241	1243	rBV	38772	36779	1.36%	0.135%
19	9.445	1247	1251	1255	rVB	455585	375234	13.87%	1.373%
20	9.586	1272	1275	1278	rVB	47900	37002	1.37%	0.135%
21	9.663	1285	1288	1292	rVB	46309	36783	1.36%	0.135%
22	9.727	1292	1299	1302	rVV	930192	822981	30.41%	3.012%
23	9.757	1302	1304	1308	rVB2	27409	28196	1.04%	0.103%
24	9.927	1330	1333	1336	rBV	41939	37910	1.40%	0.139%
25	10.133	1364	1368	1370	rBV	32381	31952	1.18%	0.117%
26	10.163	1370	1373	1375	rVB	55969	47303	1.75%	0.173%
27	10.427	1416	1418	1422	rVB4	25004	27071	1.00%	0.099%
28	10.515	1427	1433	1436	rBV	1483813	1387873	51.29%	5.080%
29	10.545	1436	1438	1445	rVB3	42921	47799	1.77%	0.175%
30	10.633	1450	1453	1461	rBV2	103960	148540	5.49%	0.544%
31	11.080	1526	1529	1531	rBV	69622	55096	2.04%	0.202%
32	11.110	1531	1534	1541	rVB2	43979	50724	1.87%	0.186%
33	11.210	1547	1551	1553	rBV	899130	778875	28.78%	2.851%
34	11.233	1553	1555	1558	rVV	205466	162527	6.01%	0.595%

LSC Area Percent Report

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Data File : BF098330.D
Acq On : 7 Sep 2017 22:58
Operator : SJ/JU
Sample : I5071-08
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G58A-2.5-5

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-BF081517.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	11.280	1558	1563	1567	rVB	80963	100001	3.70%	0.366%
36	11.504	1599	1601	1604	rBV	55100	43448	1.61%	0.159%
37	11.710	1633	1636	1638	rBV	50885	41781	1.54%	0.153%
38	11.739	1638	1641	1644	rVB	83565	72214	2.67%	0.264%
39	11.786	1644	1649	1651	rBV2	28789	36246	1.34%	0.133%
40	11.815	1651	1654	1657	rVV	77544	93131	3.44%	0.341%
41	11.845	1657	1659	1663	rVB	42927	38236	1.41%	0.140%
42	11.915	1668	1671	1673	rVB	45126	38364	1.42%	0.140%
43	12.004	1684	1686	1689	rBV	41375	35413	1.31%	0.130%
44	12.257	1726	1729	1732	rBV	66814	65809	2.43%	0.241%
45	12.298	1732	1736	1741	rVV3	57004	79094	2.92%	0.289%
46	12.345	1741	1744	1748	rVV	53874	52933	1.96%	0.194%
47	12.421	1753	1757	1760	rBV	363668	346942	12.82%	1.270%
48	12.645	1789	1795	1798	rBV	383036	413667	15.29%	1.514%
49	12.668	1798	1799	1802	rVV2	46203	36467	1.35%	0.133%
50	12.698	1802	1804	1809	rVB3	33150	38431	1.42%	0.141%
51	12.798	1816	1821	1824	rBV	2302773	2199428	81.28%	8.050%
52	12.862	1830	1832	1836	rBV2	34351	46346	1.71%	0.170%
53	12.951	1845	1847	1849	rBV2	41560	52421	1.94%	0.192%
54	12.974	1849	1851	1854	rVB	67634	59886	2.21%	0.219%
55	13.009	1854	1857	1858	rBV2	30974	30485	1.13%	0.112%
56	13.080	1865	1869	1871	rBV2	64451	72438	2.68%	0.265%
57	13.204	1887	1890	1893	rBV	30588	31553	1.17%	0.115%
58	13.280	1897	1903	1909	rBV	909502	898941	33.22%	3.290%
59	13.333	1910	1912	1914	rBV	37498	36161	1.34%	0.132%
60	13.486	1935	1938	1942	rVB	63669	69817	2.58%	0.256%
61	13.692	1970	1973	1978	rBV	232021	244152	9.02%	0.894%
62	13.845	1994	1999	2002	rBV2	799543	924071	34.15%	3.382%
63	13.868	2002	2003	2006	rVB	185265	108837	4.02%	0.398%
64	14.856	2167	2171	2174	rBV	169223	249013	9.20%	0.911%
65	15.139	2216	2219	2224	rVB	96840	114691	4.24%	0.420%
66	15.198	2226	2229	2234	rVB	99739	121851	4.50%	0.446%
67	15.256	2235	2239	2242	rBV	408547	451762	16.69%	1.653%

Sum of corrected areas: 27322339

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Acq On : 7 Sep 2017 22:58
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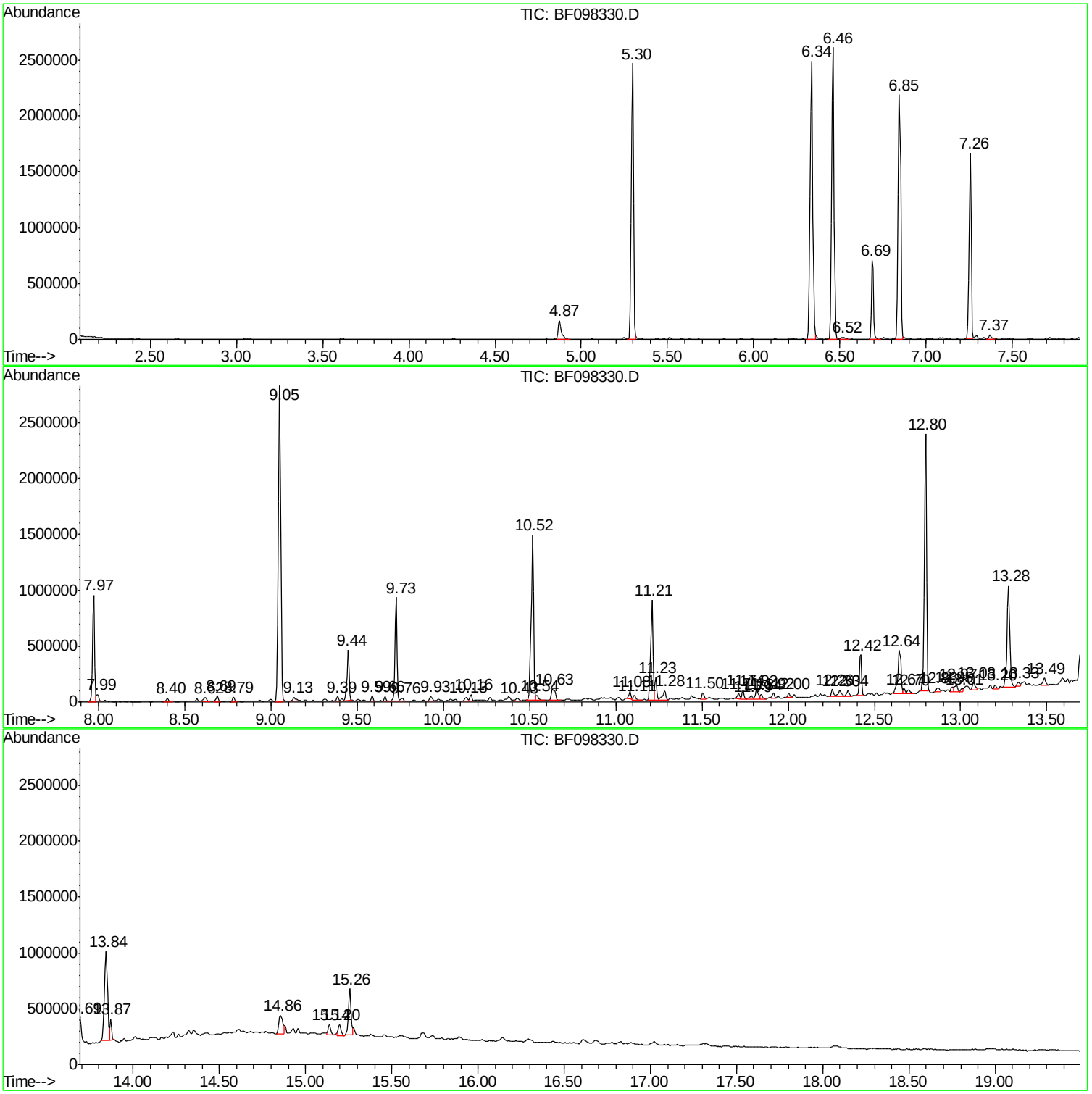
Sample : I5071-08
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
G58A-2.5-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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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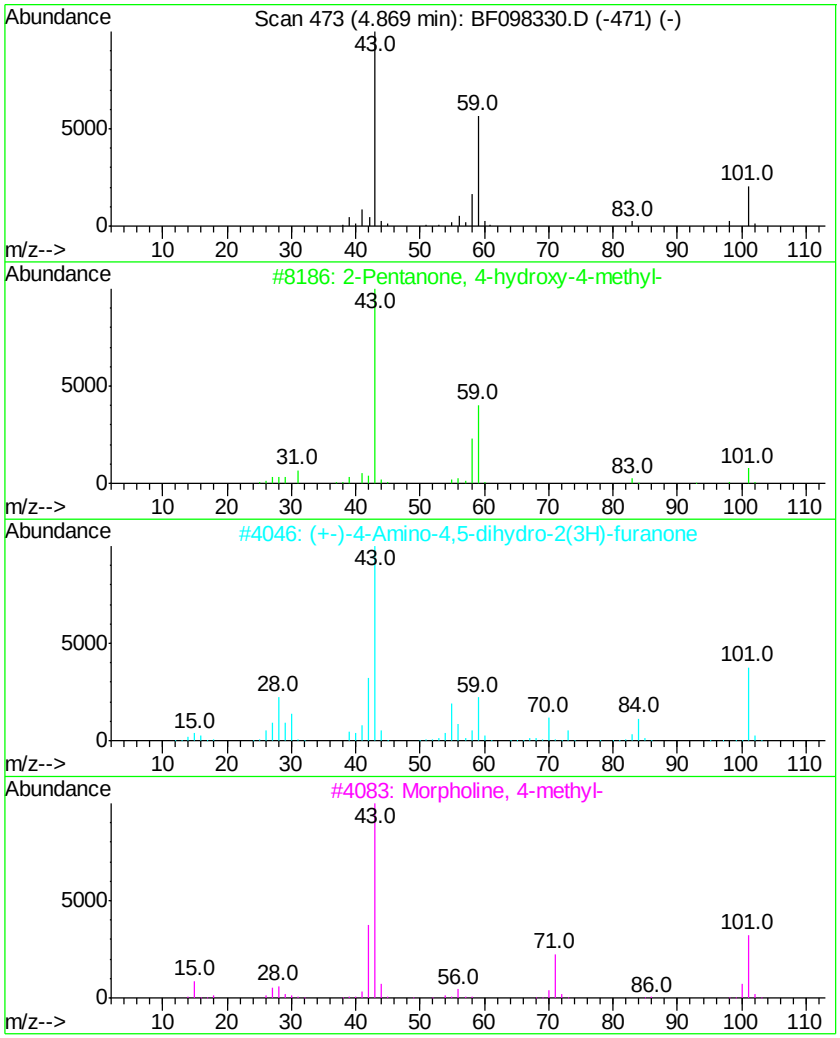
TIC Integration Parameters: LSCINT.P

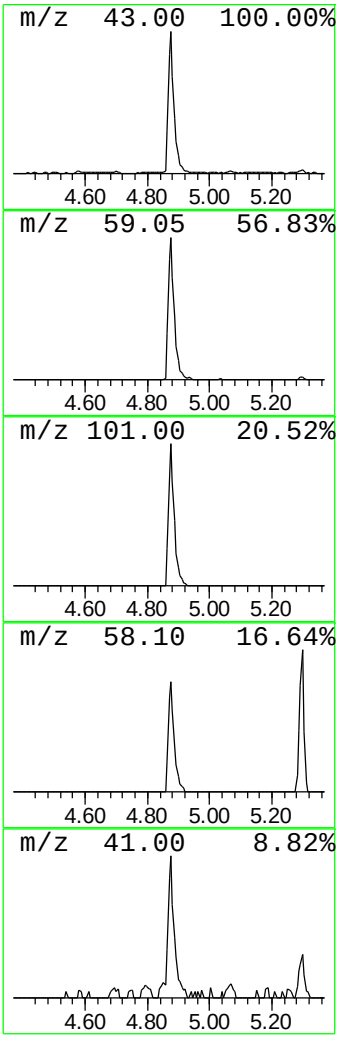
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.87	7.07 ng	222546	1,4-Dichlorobenzene-d4	6.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





Library Search Compound Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF090717\
Data File : BF098330.D
Acq On : 7 Sep 2017 22:58
Operator : SJ/JU
Sample : I5071-08
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G58A-2.5-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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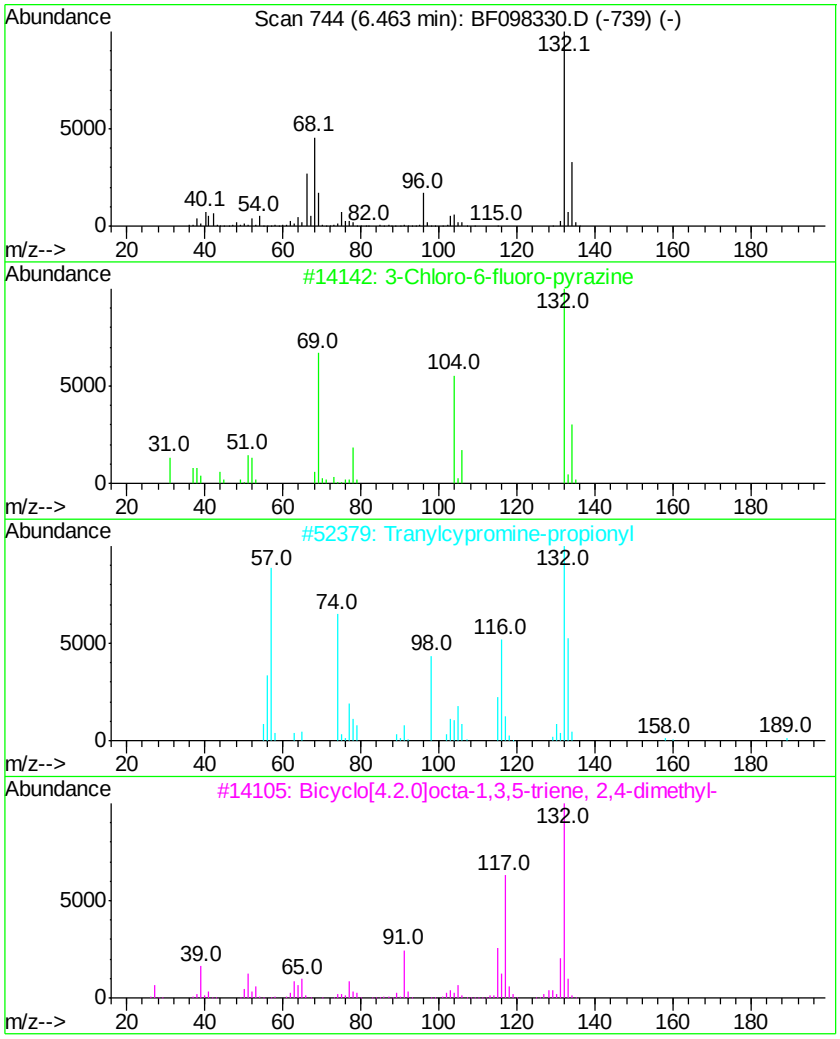
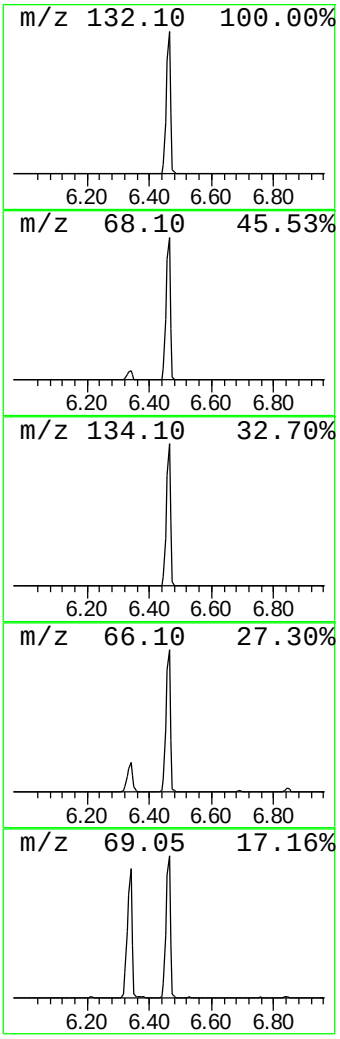
****

Peak Number 2 unknown6.46 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.46	80.07 ng	2519380	1,4-Dichlorobenzene-d4	6.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





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ClientSampleId : G58A-2.5-5

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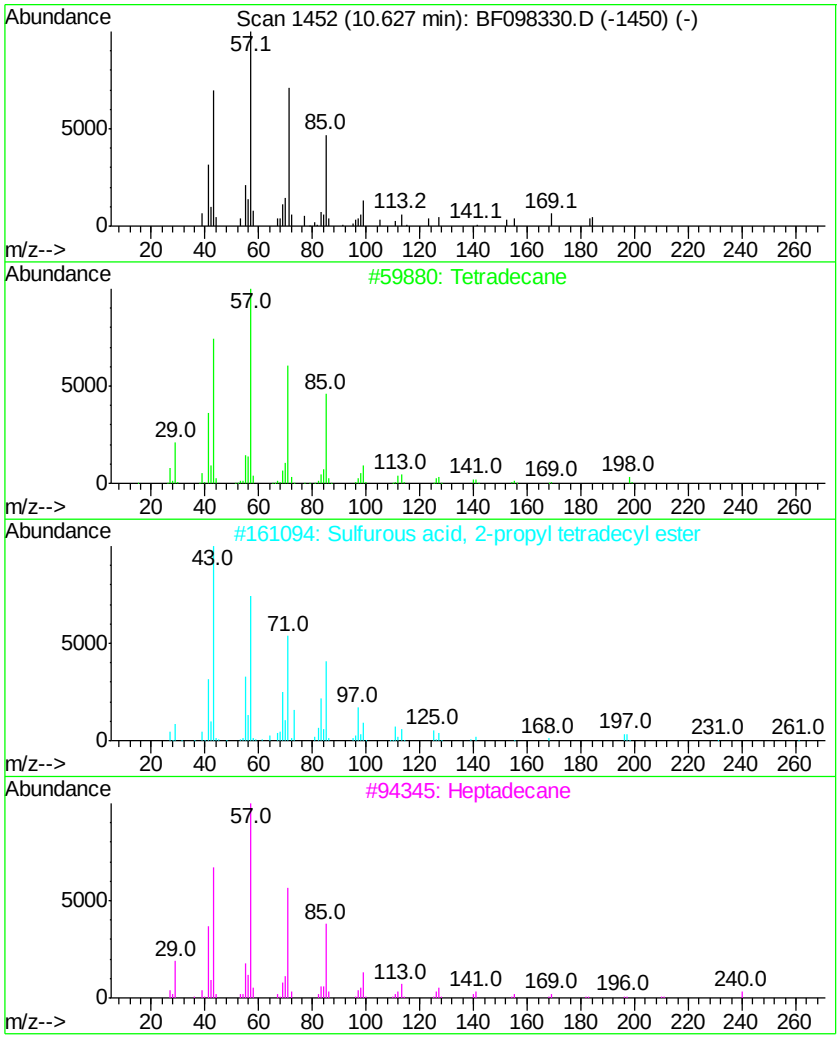
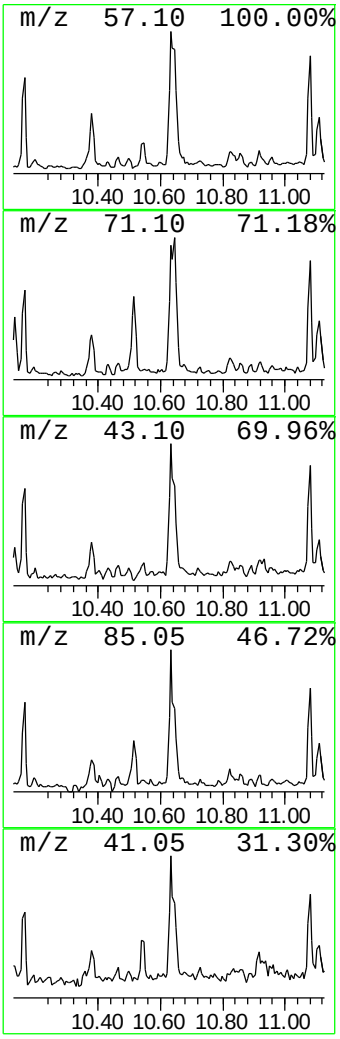
****

Peak Number 4 Tetradecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.63	3.81 ng	148540	Phenanthrene-d10	11.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane	198	C14H30	000629-59-4	87
2	Sulfurous acid, 2-propyl tetrade...	320	C17H36O3S	1000309-12-5	86
3	Heptadecane	240	C17H36	000629-78-7	83
4	Undecane, 2-methyl-	170	C12H26	007045-71-8	80
5	Undecane, 5-methyl-	170	C12H26	001632-70-8	80





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Instrument : BNA_F
ClientSampleId : G58A-2.5-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
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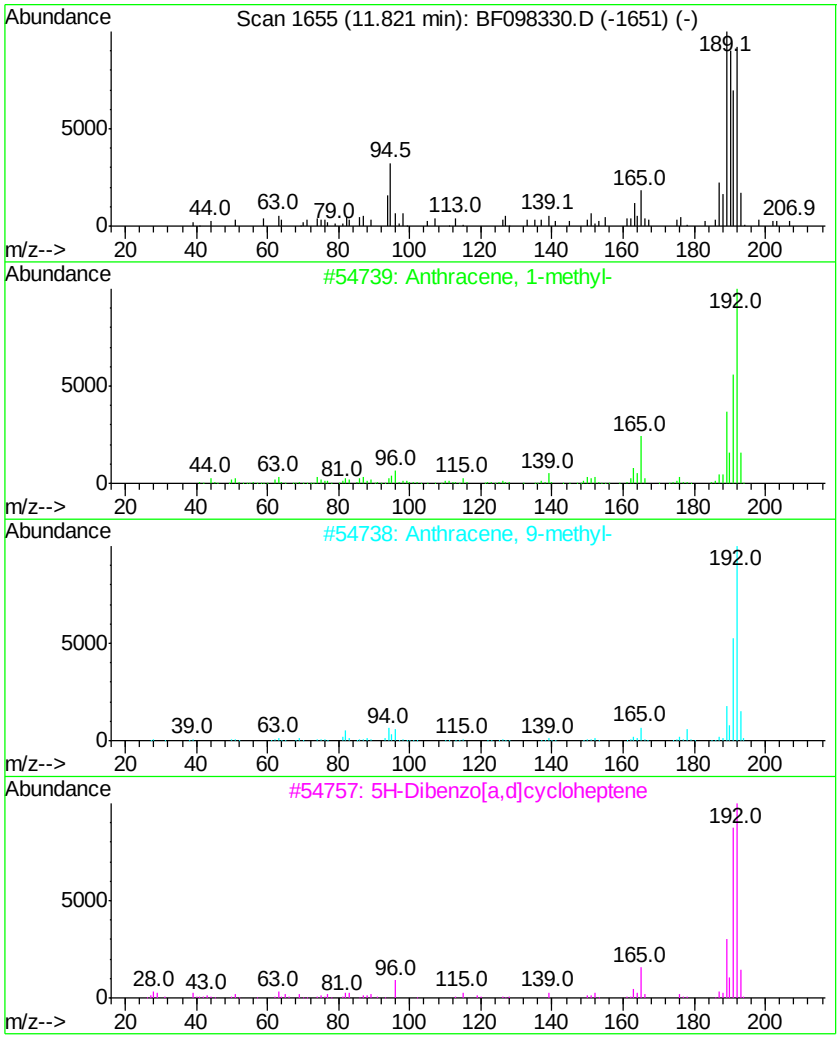
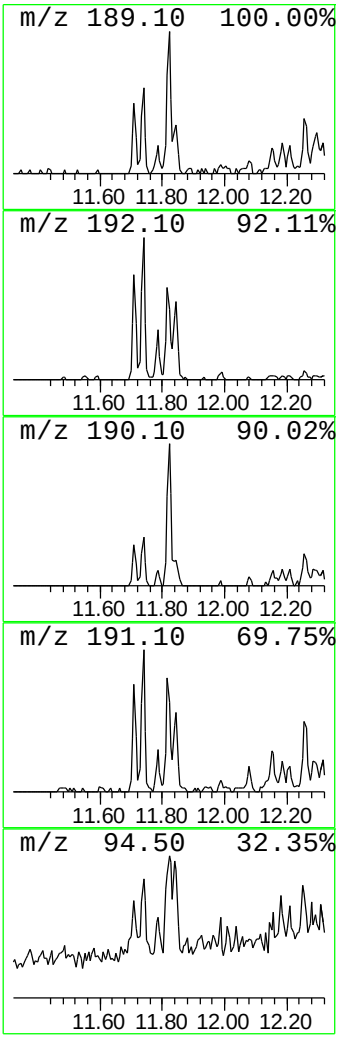
****

Peak Number 5 Anthracene, 1-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.82	2.39 ng	93131	Phenanthrene-d10	11.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 1-methyl-	192	C15H12	000610-48-0	83
2	Anthracene, 9-methyl-	192	C15H12	000779-02-2	70
3	5H-Dibenzo[a,d]cycloheptene	192	C15H12	000256-81-5	64
4	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	64
5	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	64





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Misc :
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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

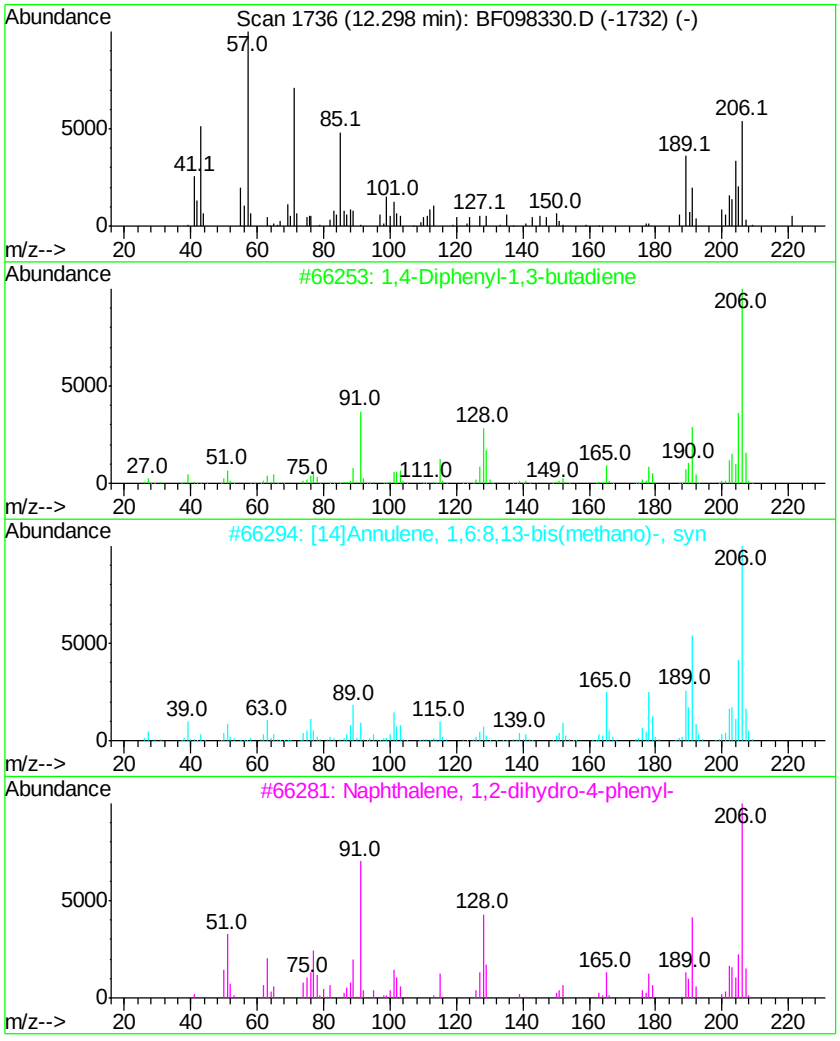
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

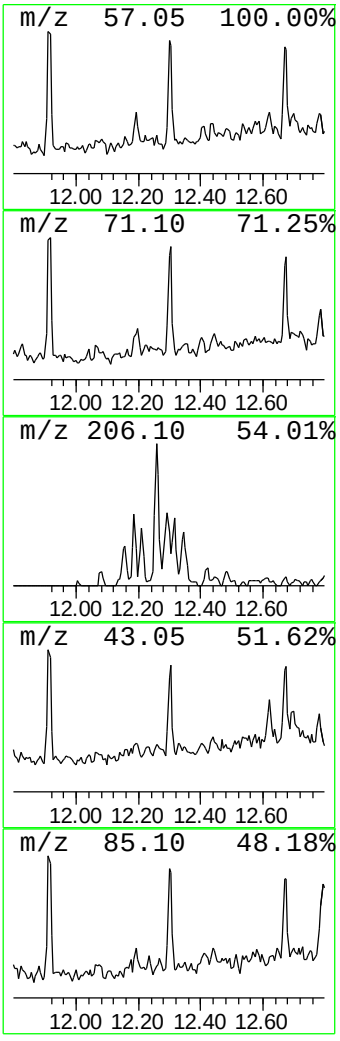
****

Peak Number 6 unknown12.30 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.30	2.03 ng	79094	Phenanthrene-d10	11.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Diphenyl-1,3-butadiene	206	C16H14	000886-65-7	38
2	[14]Annulene, 1,6:8,13-bis(metha...	206	C16H14	085385-68-8	35
3	Naphthalene, 1,2-dihydro-4-phenyl-	206	C16H14	007469-40-1	30
4	1,3-Butadiene, 1,4-diphenyl-, (E...	206	C16H14	000538-81-8	27
5	Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	25





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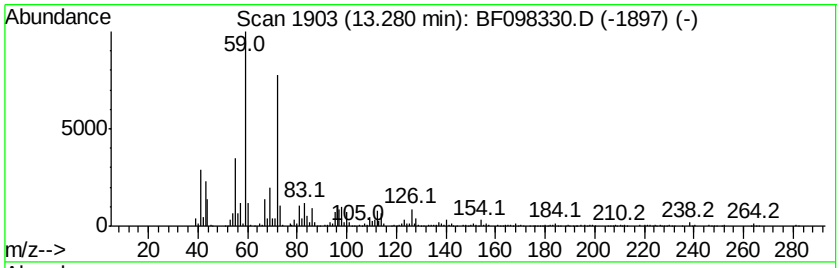
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

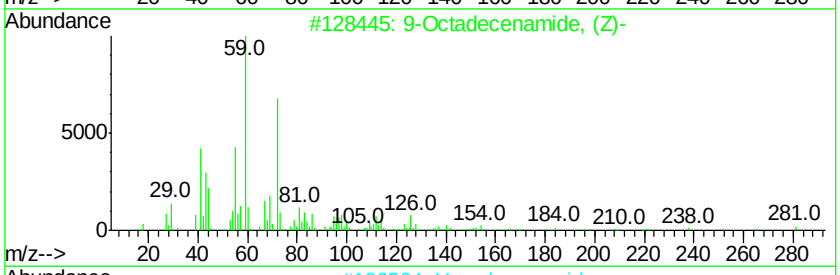
****

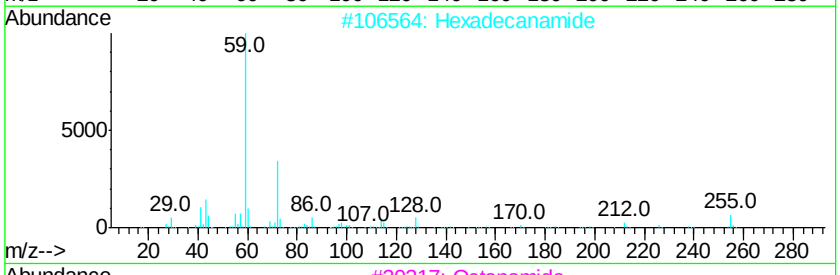
Peak Number 7 9-Octadecenamide, (Z)- Concentration Rank 3

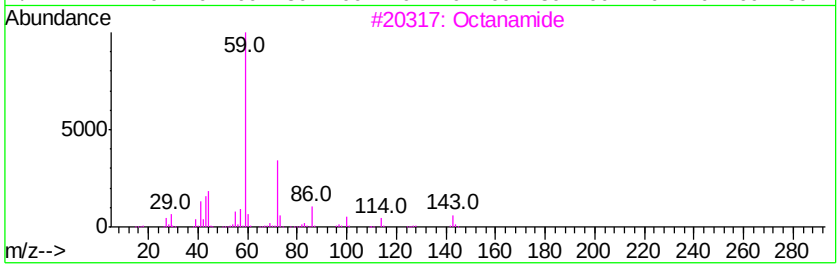
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.28	19.46 ng	898941	Chrysene-d12	13.84

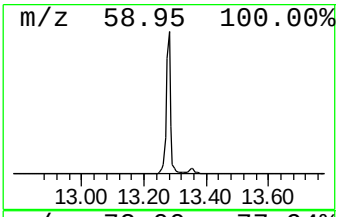
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
2	Hexadecanamide	255	C16H33NO	000629-54-9	59
3	Octanamide	143	C8H17NO	000629-01-6	43
4	2-Ethoxyethyl heptanoate	202	C11H22O3	1000367-02-0	43
5	Dodecanamide	199	C12H25NO	001120-16-7	38

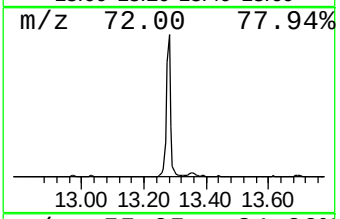


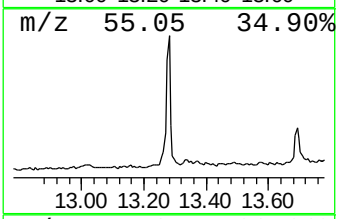


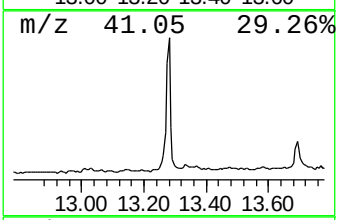


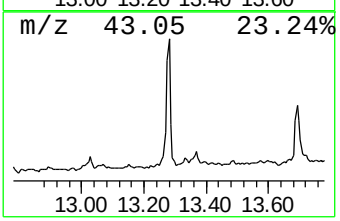












Library Search Compound Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF090717\
Data File : BF098330.D
Acq On : 7 Sep 2017 22:58
Operator : SJ/JU
Sample : I5071-08
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G58A-2.5-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

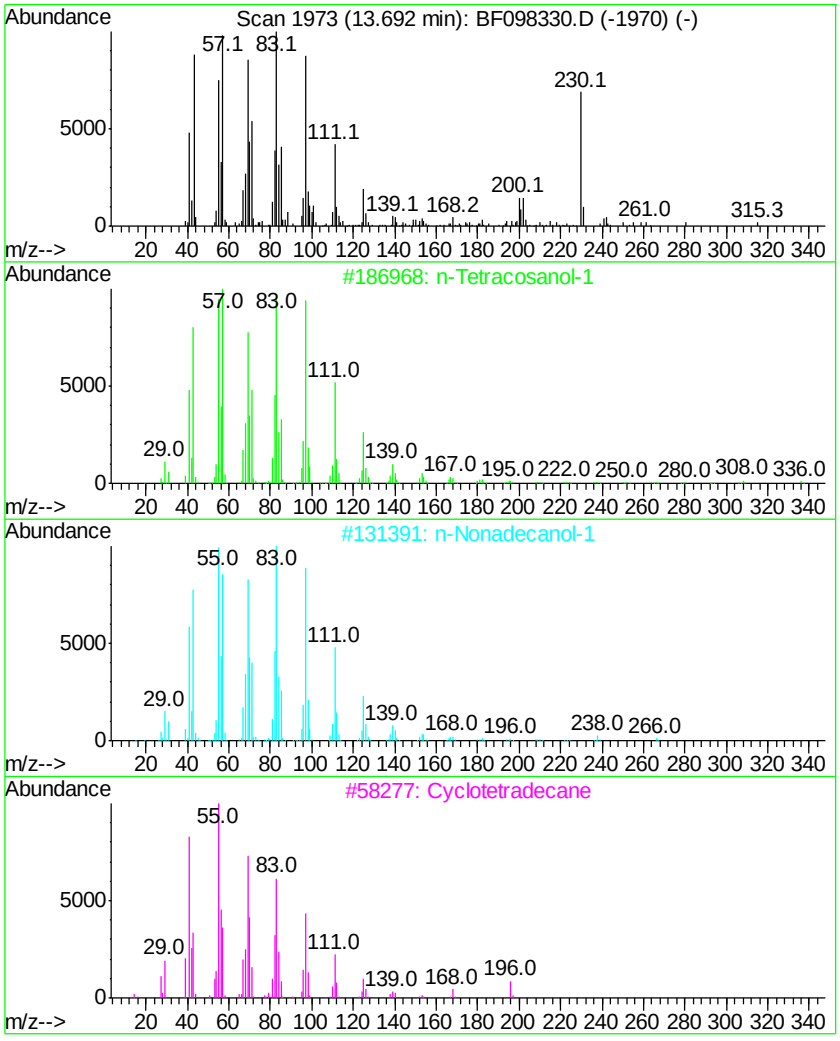
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

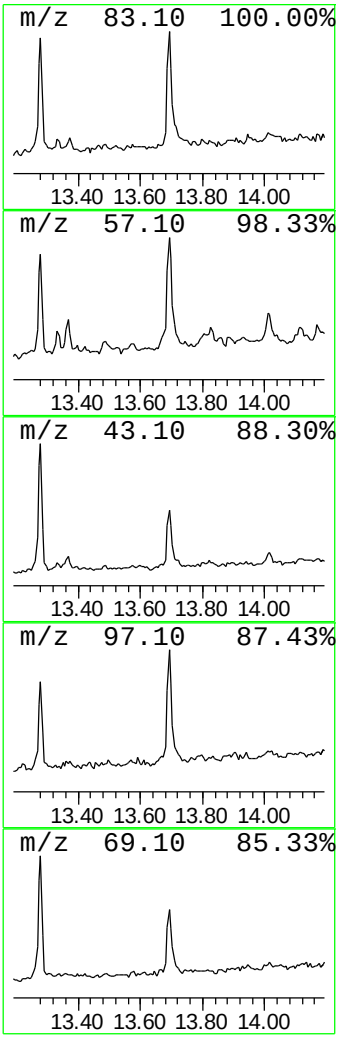
****

Peak Number 8 n-Tetracosanol-1 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.69	5.28 ng	244152	Chrysene-d12	13.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	87
2	n-Nonadecanol-1	284	C19H40O	001454-84-8	81
3	Cyclotetradecane	196	C14H28	000295-17-0	74
4	9-Eicosene, (E)-	280	C20H40	074685-29-3	68
5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	55





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Data File : BF098330.D
Acq On : 7 Sep 2017 22:58
Operator : SJ/JU
Sample : I5071-08
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G58A-2.5-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

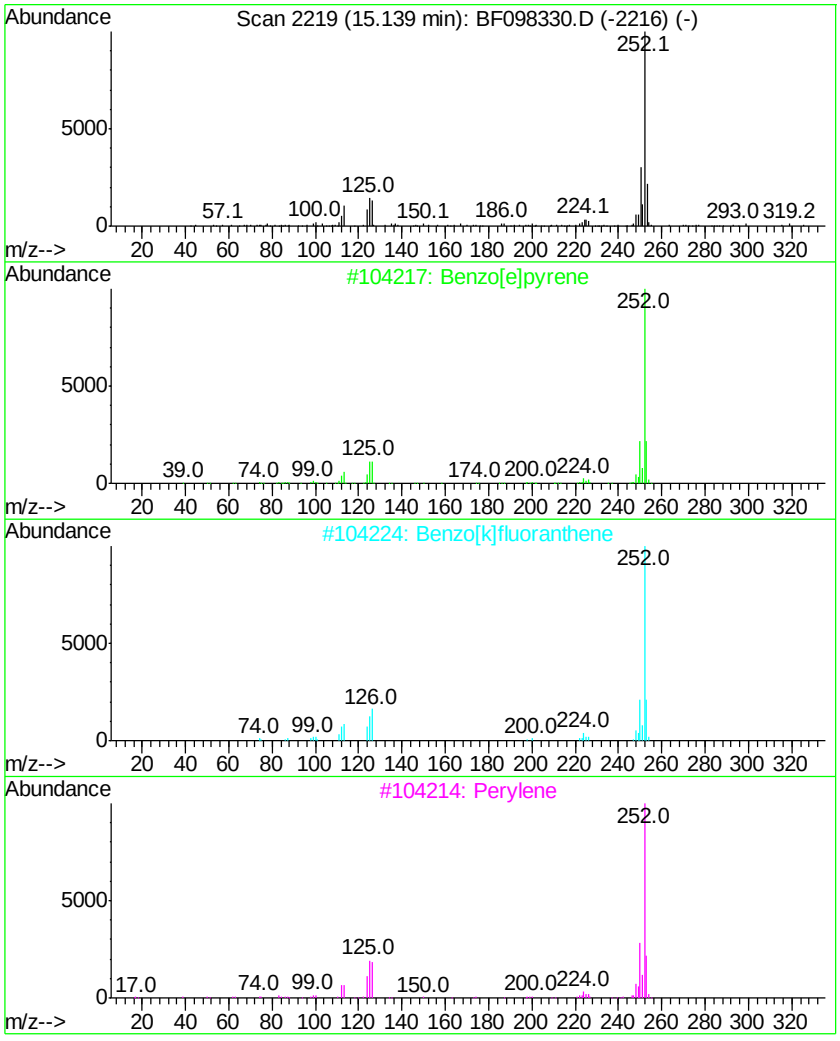
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

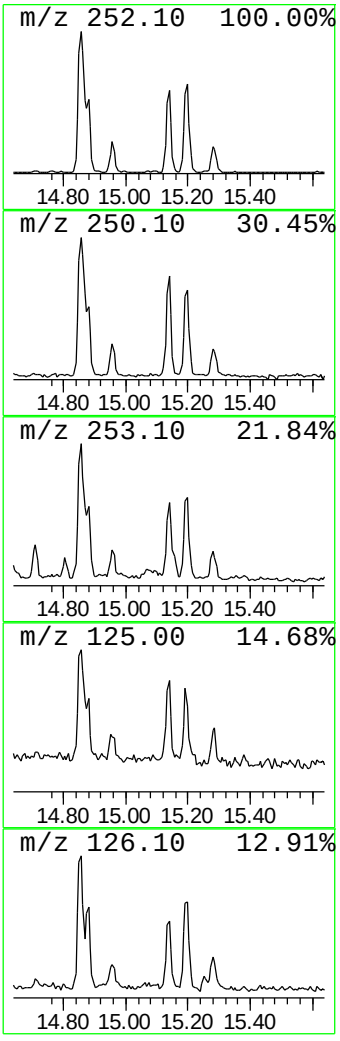
****

Peak Number 9 Benzo[e]pyrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.14	5.08 ng	114691	Perylene-d12	15.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	99
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	98
3	Perylene	252	C20H12	000198-55-0	98
4	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	96
5	Benzo[a]pyrene	252	C20H12	000050-32-8	93





Tentatively Identified Compound (LSC) summary

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_F\DATA\BF090717\
Data File : BF098330.D
Acq On : 7 Sep 2017 22:58
Operator : SJ/JU
Sample : I5071-08
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G58A-2.5-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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...	4.87	7.1	ng	222546	1	6.69	629326	20.0
unknown6.46	6.46	80.1	ng	2519380	1	6.69	629326	20.0
Tetradecane	10.63	3.8	ng	148540	4	11.21	778875	20.0
Anthracene, 1-met...	11.82	2.4	ng	93131	4	11.21	778875	20.0
unknown12.30	12.30	2.0	ng	79094	4	11.21	778875	20.0
9-Octadecenamide,...	13.28	19.5	ng	898941	5	13.84	924071	20.0
n-Tetracosanol-1	13.69	5.3	ng	244152	5	13.84	924071	20.0
Benzo[e]pyrene	15.14	5.1	ng	114691	6	15.26	451762	20.0