LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF090717\
Data File : BF098335.D
Acq On : 8 Sep 2017 1:18
Operator : SJ/JU
Sample : I5071-14
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G55A-2.5-4.5

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	3.622	256	261	269	rVB	69472	106700	3.57%	0.362%
2	4.340	379	383	388	rBV	75666	88664	2.97%	0.301%
3	4.881	472	475	490	rVB	183691	271190	9.07%	0.921%
4	5.304	542	547	550	rBV	2405922	2687520	89.90%	9.127%
5	6.340	718	723	726	rBV	2441647	2936967	98.25%	9.974%
6	6.463	739	744	747	rBV	2804220	2741340	91.70%	9.309%
7	6.516	750	753	760	rVB2	22637	35823	1.20%	0.122%
8	6.692	779	783	790	rVB	731353	686418	22.96%	2.331%
9	6.845	805	809	813	rBV	2217720	2104471	70.40%	7.147%
10	7.257	874	879	882	rBV	1606324	1719352	57.52%	5.839%
11	7.292	882	885	888	rVB2	32494	33174	1.11%	0.113%
12	7.375	895	899	908	rVB	61880	74553	2.49%	0.253%
13	7.975	996	1001	1003	rBV	985439	885183	29.61%	3.006%
14	7.992	1003	1004	1007	rVB	77383	50159	1.68%	0.170%
15	8.398	1069	1073	1077	rBV	50062	47368	1.58%	0.161%
16	8.569	1099	1102	1106	rVB	44072	33833	1.13%	0.115%
17	8.686	1119	1122	1125	rVB	75430	57497	1.92%	0.195%
18	8.786	1135	1139	1142	rBV	50539	40685	1.36%	0.138%
19	9.051	1179	1184	1187	rBV	2981978	2989318	100.00%	10.152%
20	9.133	1192	1198	1203	rBV3	54279	69166	2.31%	0.235%
21	9.316	1225	1229	1232	rVB	24353	31445	1.05%	0.107%
22	9.386	1238	1241	1243	rBV	49599	44124	1.48%	0.150%
23	9.445	1247	1251	1255	rVV	513107	427235	14.29%	1.451%
24	9.586	1272	1275	1279	rVB	69733	52832	1.77%	0.179%
25	9.663	1285	1288	1292	rVB	59417	47548	1.59%	0.161%
26	9.728	1292	1299	1302	rBV	968795	868394	29.05%	2.949%
27	9.928	1330	1333	1337	rBV	49648	48053	1.61%	0.163%
28	9.969	1337	1340	1345	rVB3	24259	32877	1.10%	0.112%
29	10.133	1364	1368	1370	rBV	39921	41600	1.39%	0.141%
30	10.163	1370	1373	1377	rVB	70468	61448	2.06%	0.209%
31	10.380	1404	1410	1415	rBV2	44034	58105	1.94%	0.197%
32	10.516	1427	1433	1436	rVV	1455957	1403242	46.94%	4.765%
33	10.539	1436	1437	1444	rVB3	39710	48947	1.64%	0.166%
34	10.633	1450	1453	1459	rBV3	116497	167782	5.61%	0.570%

LSC Area Percent Report

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Operator : SJ/JU
Sample : I5071-14
Misc :
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Instrument : BNA_F
ClientSampleId : G55A-2.5-4.5

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

35	11.016	1515	1518	1522	rBV3	32078	30532	1.02%	0.104%
36	11.080	1526	1529	1531	rVV	90619	82253	2.75%	0.279%
37	11.110	1531	1534	1540	rVB2	45969	50973	1.71%	0.173%
38	11.210	1547	1551	1553	rBV	838553	721419	24.13%	2.450%
39	11.233	1553	1555	1558	rVV	194443	152476	5.10%	0.518%
40	11.280	1558	1563	1567	rVB	69146	82503	2.76%	0.280%
41	11.445	1588	1591	1596	rBV2	31676	43630	1.46%	0.148%
42	11.504	1599	1601	1604	rVV	66449	58769	1.97%	0.200%
43	11.539	1604	1607	1613	rVB6	23382	37402	1.25%	0.127%
44	11.710	1633	1636	1638	rBV	52843	43990	1.47%	0.149%
45	11.739	1638	1641	1644	rVV	85461	76736	2.57%	0.261%
46	11.775	1644	1647	1651	rVV2	65114	70456	2.36%	0.239%
47	11.822	1651	1655	1657	rVV	71608	89969	3.01%	0.306%
48	11.845	1657	1659	1663	rVB	38845	34940	1.17%	0.119%
49	11.916	1668	1671	1673	rVB2	50862	43080	1.44%	0.146%
50	12.004	1683	1686	1689	rBV2	42936	46516	1.56%	0.158%
51	12.033	1689	1691	1696	rVB2	39114	38428	1.29%	0.130%
52	12.186	1714	1717	1719	rBV	38775	33606	1.12%	0.114%
53	12.257	1726	1729	1732	rBV	65029	69983	2.34%	0.238%
54	12.298	1733	1736	1741	rVV3	58276	82576	2.76%	0.280%
55	12.345	1741	1744	1747	rVV	43726	39983	1.34%	0.136%
56	12.422	1753	1757	1760	rBV	331519	296635	9.92%	1.007%
57	12.645	1789	1795	1798	rBV	306824	337100	11.28%	1.145%
58	12.674	1798	1800	1802	rVV	56350	47707	1.60%	0.162%
59	12.704	1802	1805	1809	rVB3	35278	48464	1.62%	0.165%
60	12.798	1816	1821	1824	rBV	2223829	2069105	69.22%	7.027%
61	12.869	1829	1833	1837	rBV4	44024	65956	2.21%	0.224%
62	12.951	1844	1847	1849	rBV2	34001	43089	1.44%	0.146%
63	13.074	1865	1868	1872	rBV2	47359	52131	1.74%	0.177%
64	13.198	1887	1889	1893	rBV	32480	35498	1.19%	0.121%
65	13.280	1898	1903	1909	rVB	520880	522080	17.46%	1.773%
66	13.333	1910	1912	1914	rBV	39814	36778	1.23%	0.125%
67	13.486	1935	1938	1942	rVB	75603	74574	2.49%	0.253%
68	13.592	1954	1956	1959	rBV	40753	31310	1.05%	0.106%
69	13.692	1970	1973	1978	rVB	153716	163591	5.47%	0.556%
70	13.845	1994	1999	2002	rBV2	781562	973200	32.56%	3.305%
71	13.868	2002	2003	2006	rVB	220086	133733	4.47%	0.454%

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Sample : I5071-14
Misc :
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Instrument : BNA_F
ClientSampleId : G55A-2.5-4.5

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
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Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

72	14.263	2068	2070	2074	rVB2	49685	52394	1.75%	0.178%
73	14.857	2167	2171	2178	rBV	277358	461019	15.42%	1.566%
74	14.927	2181	2183	2186	rVB2	78306	65807	2.20%	0.223%
75	15.139	2216	2219	2224	rVB	150602	171492	5.74%	0.582%
76	15.198	2226	2229	2234	rVB	152863	184133	6.16%	0.625%
77	15.257	2235	2239	2242	rBV	442994	545936	18.26%	1.854%
78	15.680	2308	2311	2317	rVB	84875	112091	3.75%	0.381%

Sum of corrected areas: 29447056

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Operator : SJ/JU
Sample : I5071-14
Misc :
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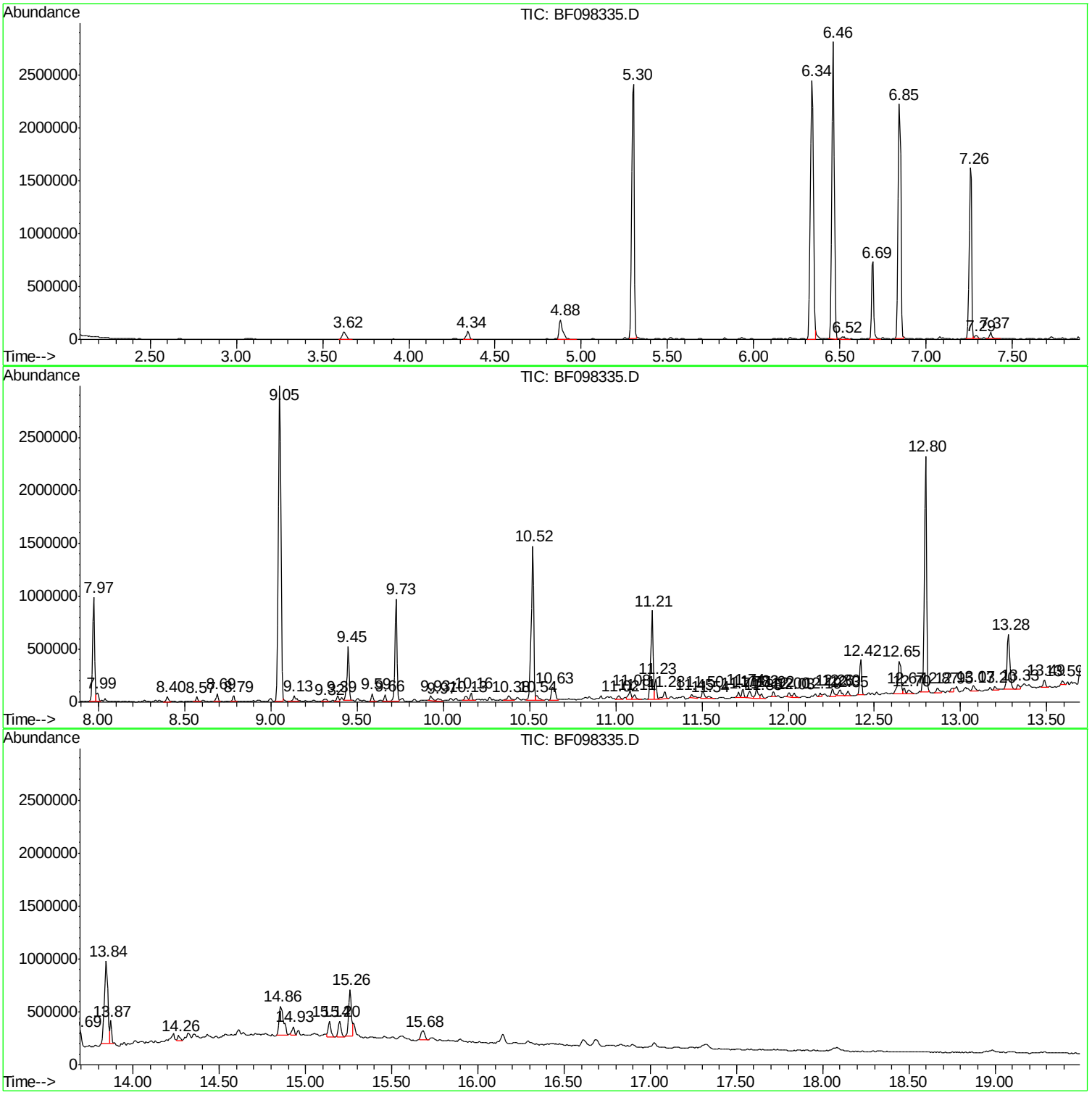
Instrument : BNA_F
ClientSampleId : G55A-2.5-4.5

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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Data File : BF098335.D
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Operator : SJ/JU
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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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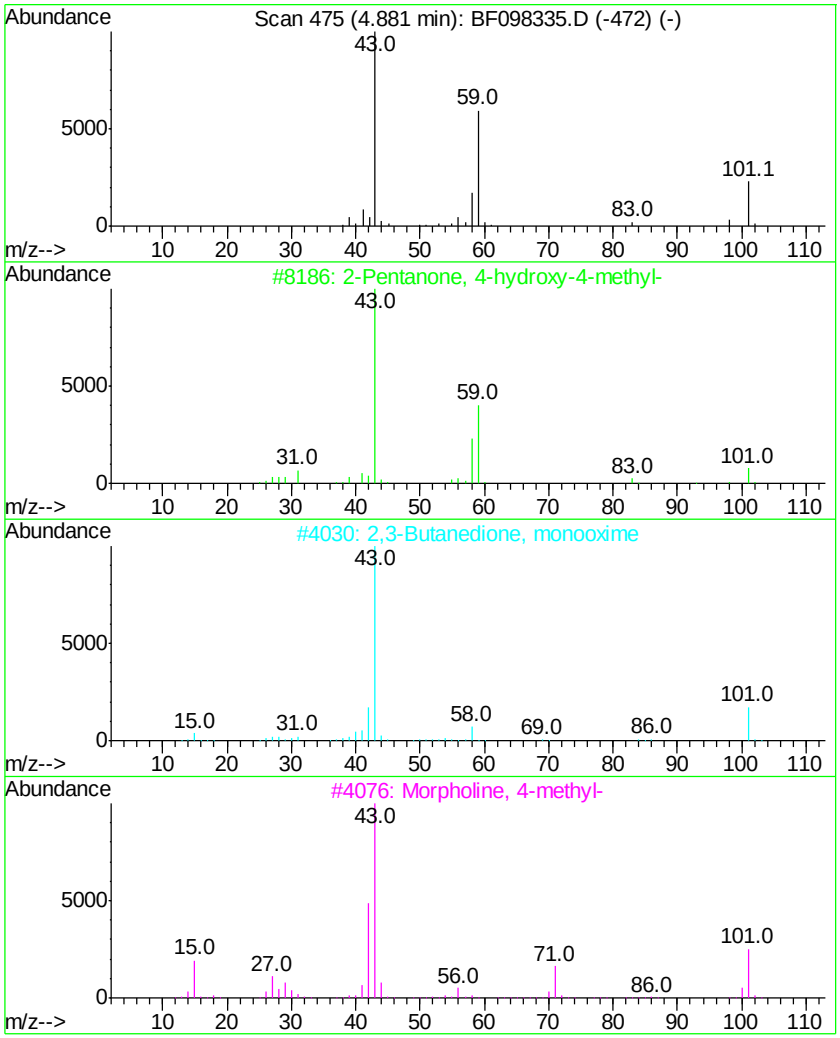
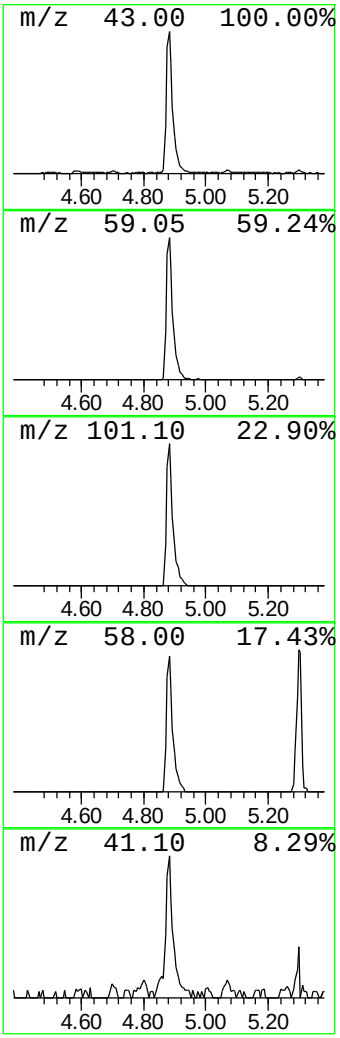
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.88	7.90 ng	271190	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	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	9
5	Propanoic acid, 2-nitro-, methyl...	133	C4H7NO4	006118-50-9	9





Library Search Compound Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF090717\
Data File : BF098335.D
Acq On : 8 Sep 2017 1:18
Operator : SJ/JU
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Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G55A-2.5-4.5

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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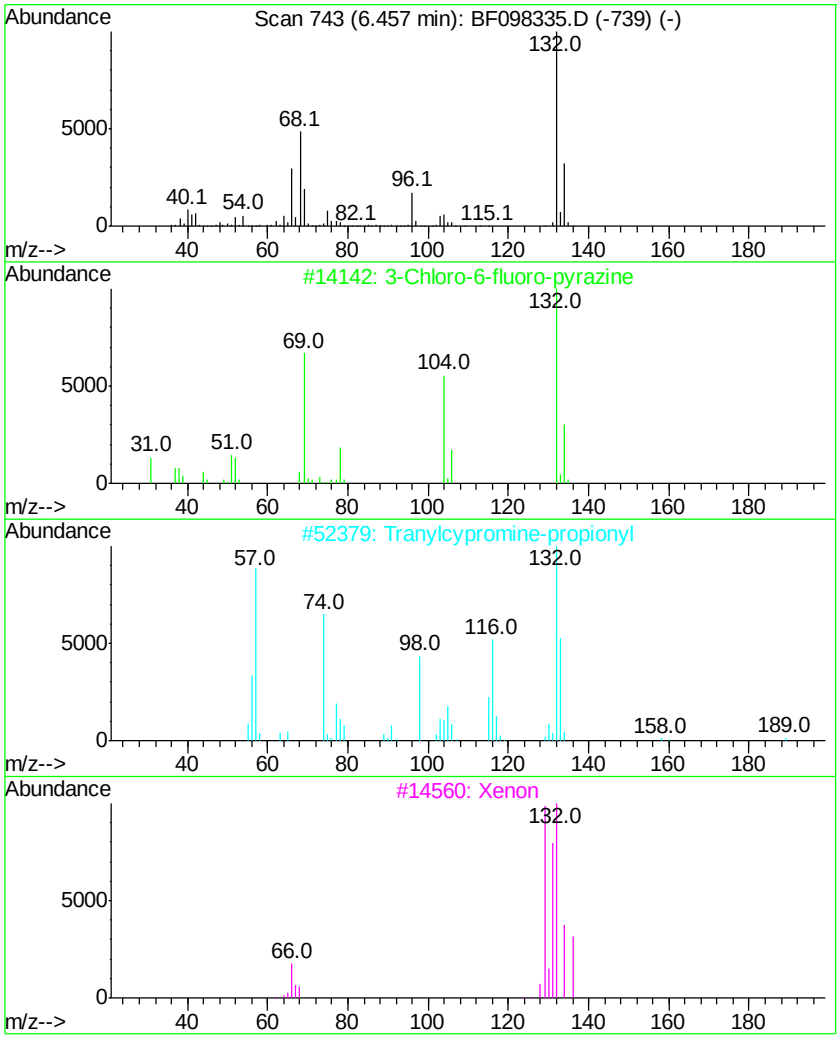
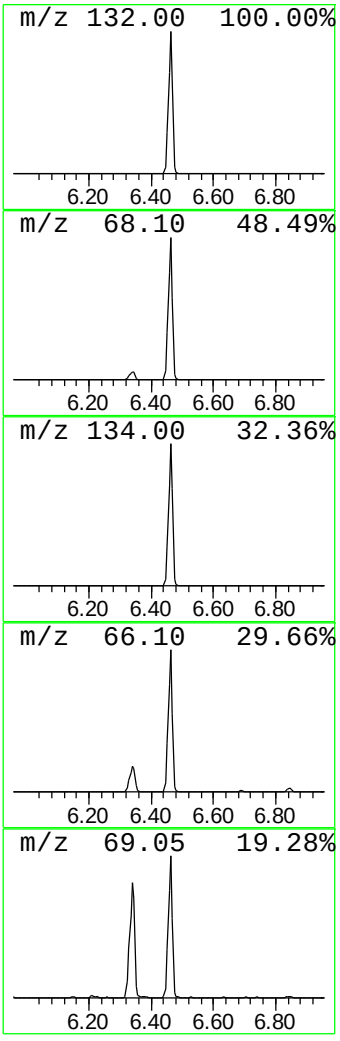
Peak Number 4 unknown6.46 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.46	79.87 ng	2741340	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	27
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	Xenon	132	Xe	007440-63-3	9
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





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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
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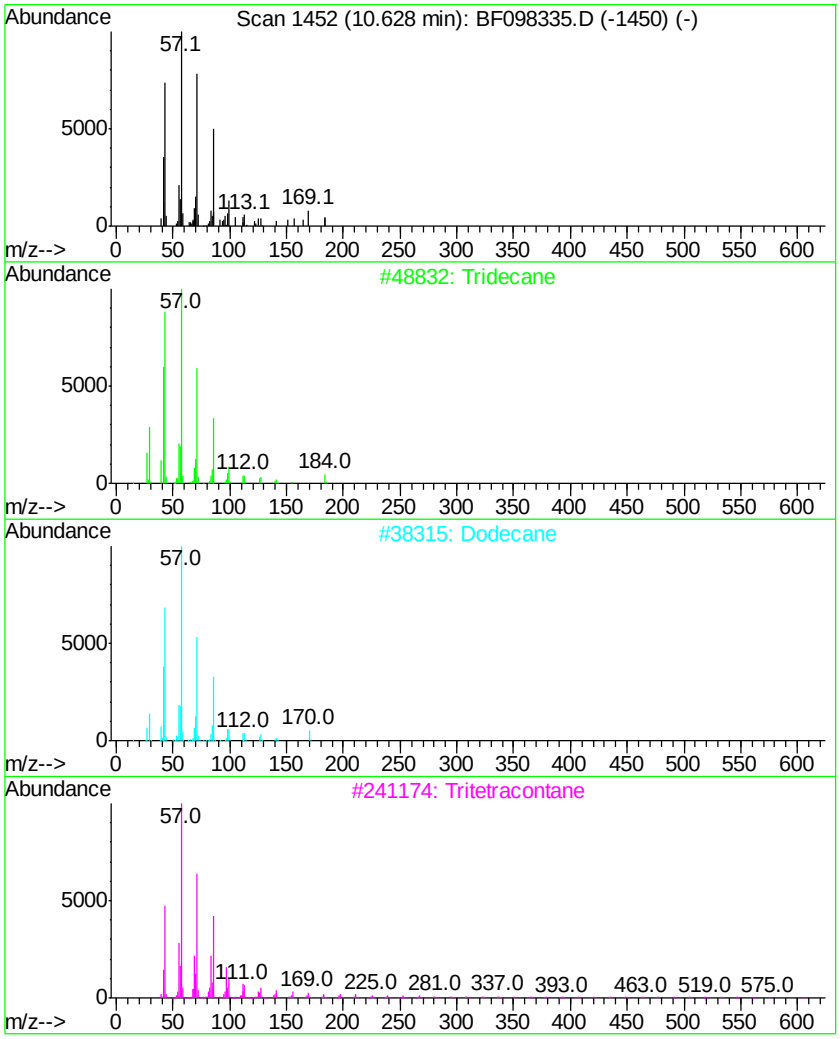
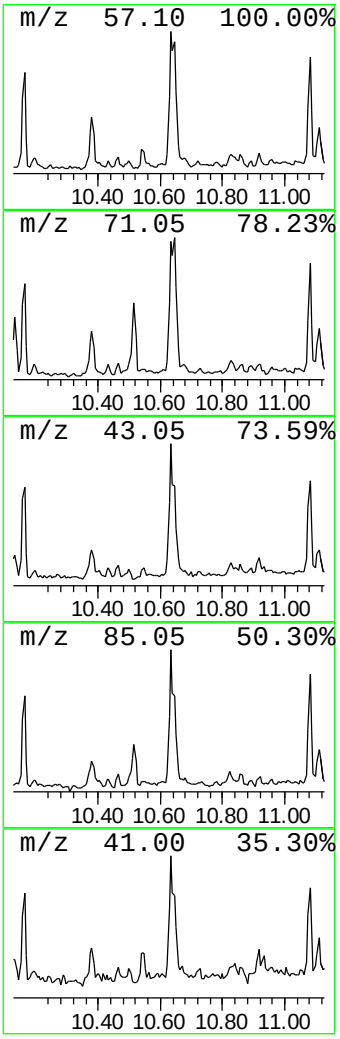
****

Peak Number 6 Tridecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.63	4.65 ng	167782	Phenanthrene-d10	11.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	87
2	Dodecane	170	C12H26	000112-40-3	83
3	Tritetracontane	605	C43H88	007098-21-7	80
4	Sulfurous acid, 2-propyl tetrade...	320	C17H36O3S	1000309-12-5	80
5	Hexadecane	226	C16H34	000544-76-3	80





Library Search Compound Report

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ClientSampleId : G55A-2.5-4.5

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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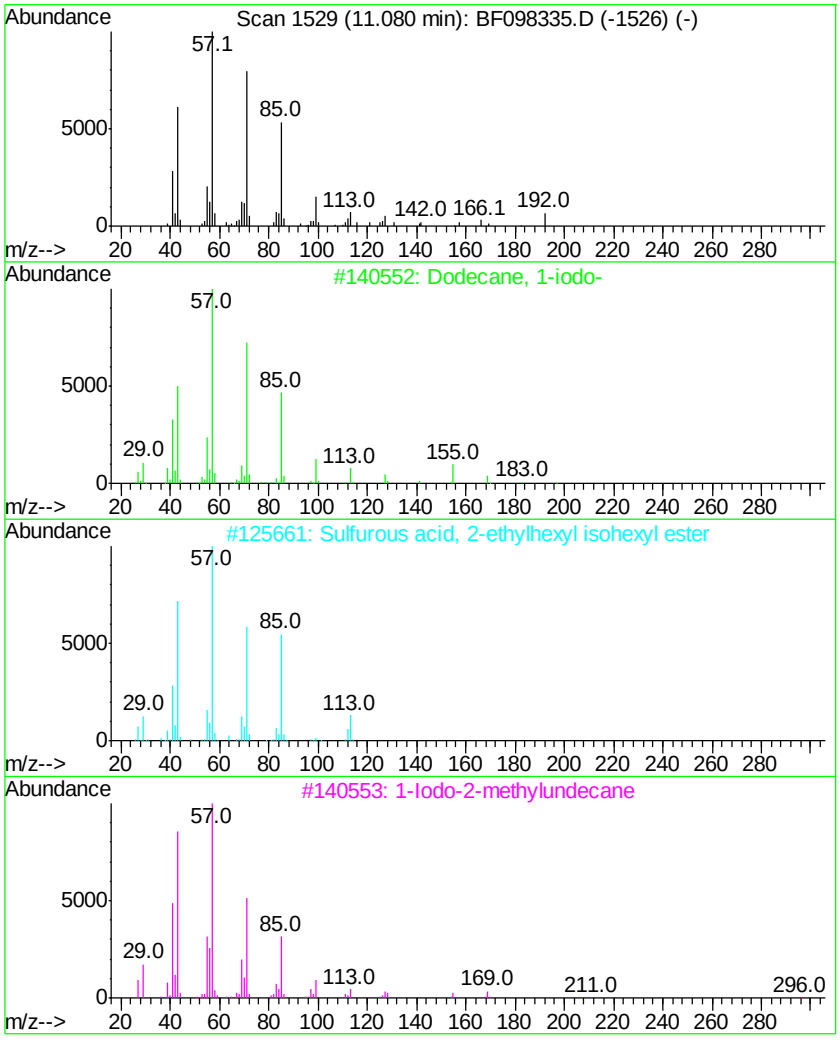
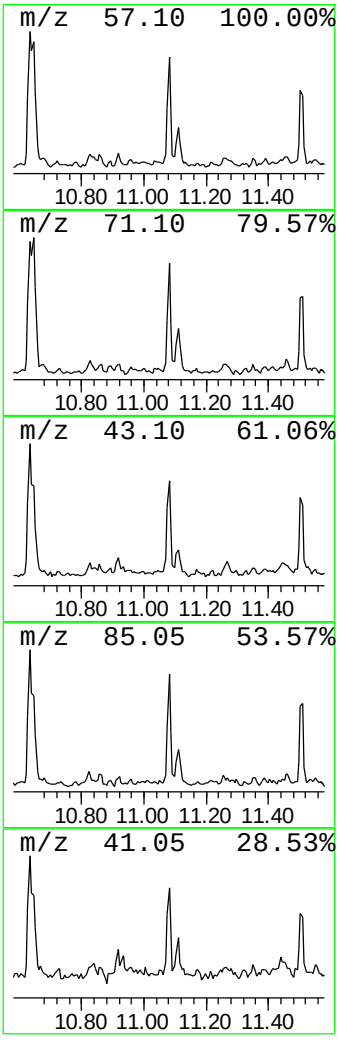
Peak Number 7 Dodecane, 1-iodo- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.08	2.28 ng	82253	Phenanthrene-d10	11.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	87
2	Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	80
3	1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	78
4	Hexadecane	226	C16H34	000544-76-3	72
5	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	72





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Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G55A-2.5-4.5

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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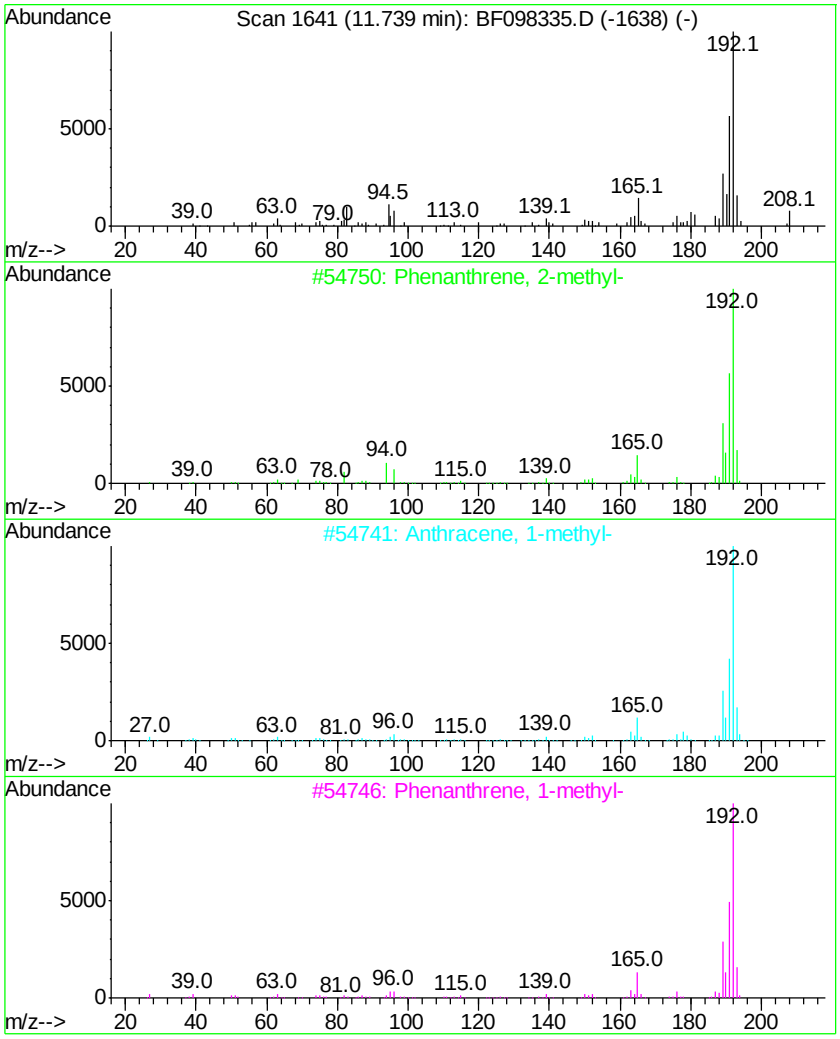
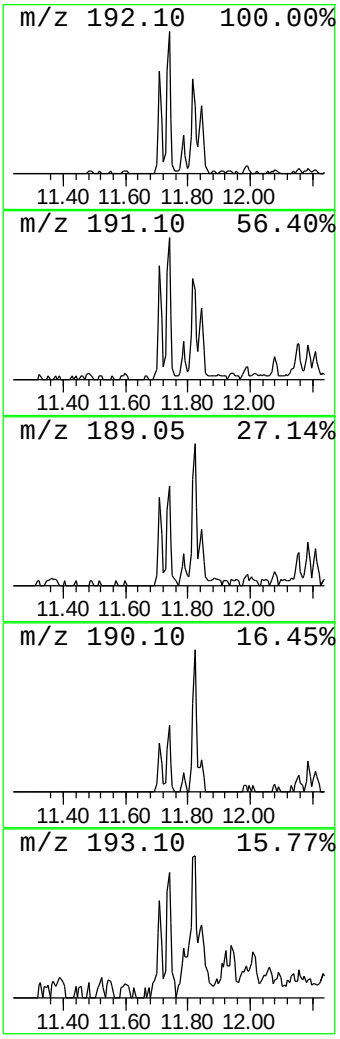
Peak Number 8 Phenanthrene, 2-methyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.74	2.13 ng	76736	Phenanthrene-d10	11.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	97
2	Anthracene, 1-methyl-	192	C15H12	000610-48-0	96
3	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	96
4	Anthracene, 2-methyl-	192	C15H12	000613-12-7	93
5	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	93





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Data File : BF098335.D
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Operator : SJ/JU
Sample : I5071-14
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G55A-2.5-4.5

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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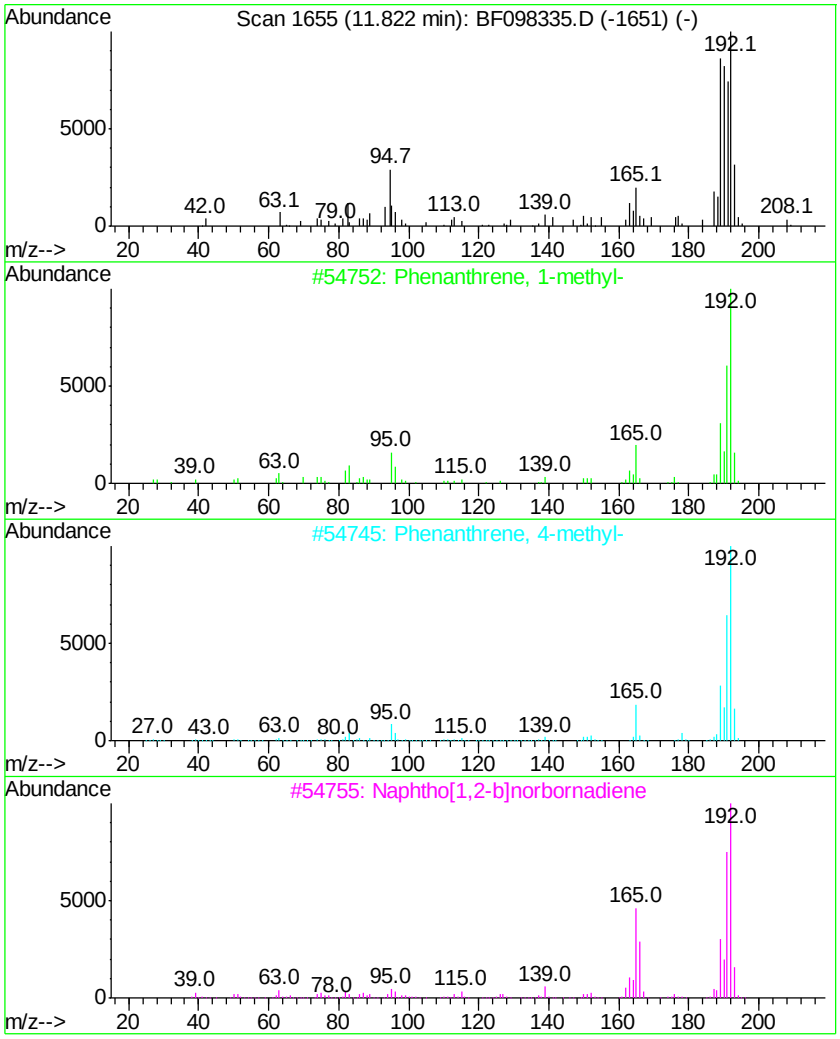
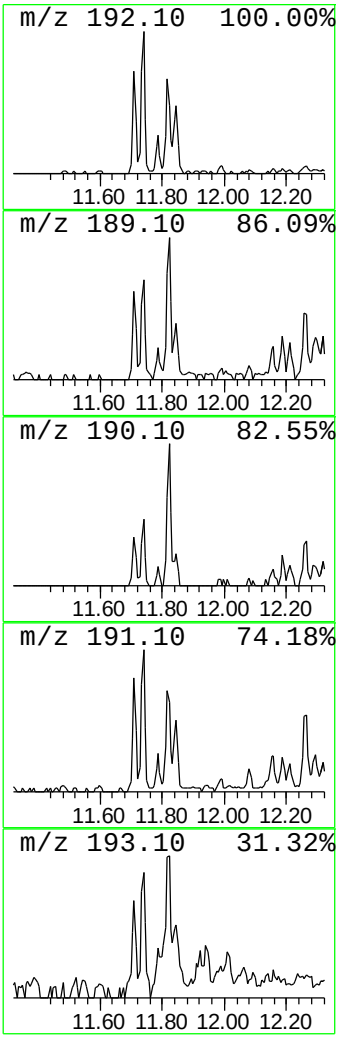
Peak Number 9 Phenanthrene, 1-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.82	2.49 ng	89969	Phenanthrene-d10	11.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	50
2	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	46
3	Naphtho[1,2-b]norbornadiene	192	C15H12	1000210-14-8	46
4	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	43
5	Anthracene, 1-methyl-	192	C15H12	000610-48-0	42





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Acq On : 8 Sep 2017 1:18
Operator : SJ/JU
Sample : I5071-14
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G55A-2.5-4.5

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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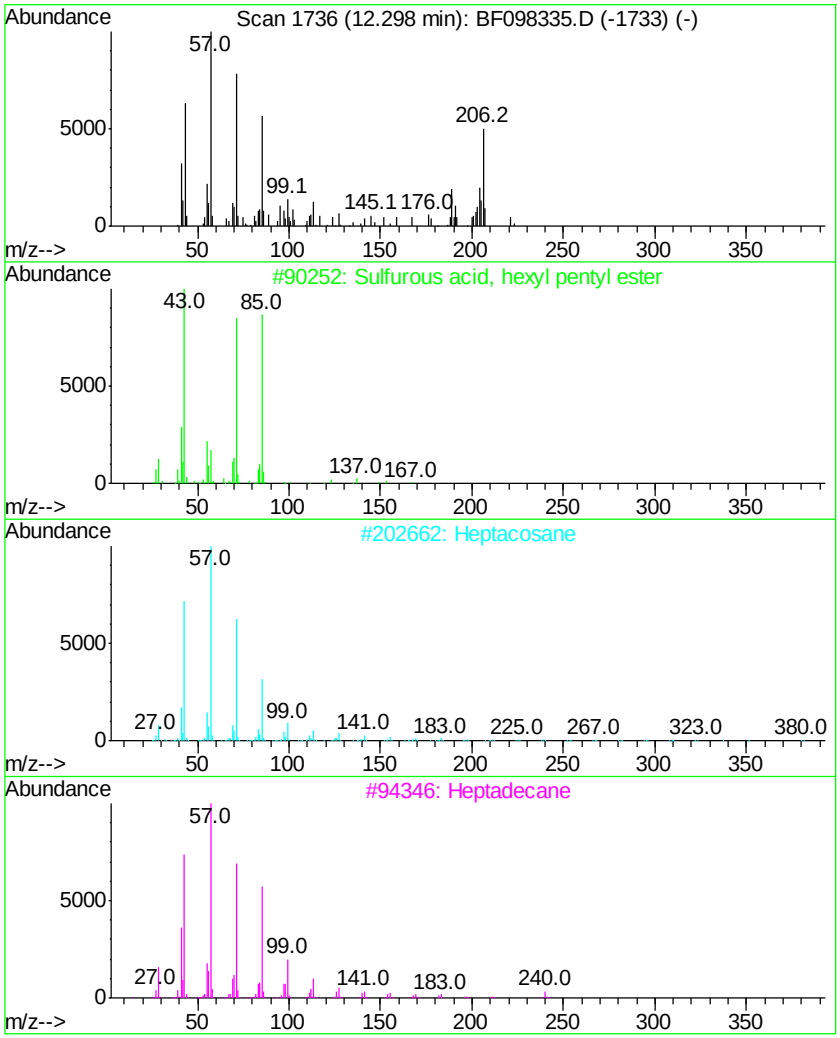
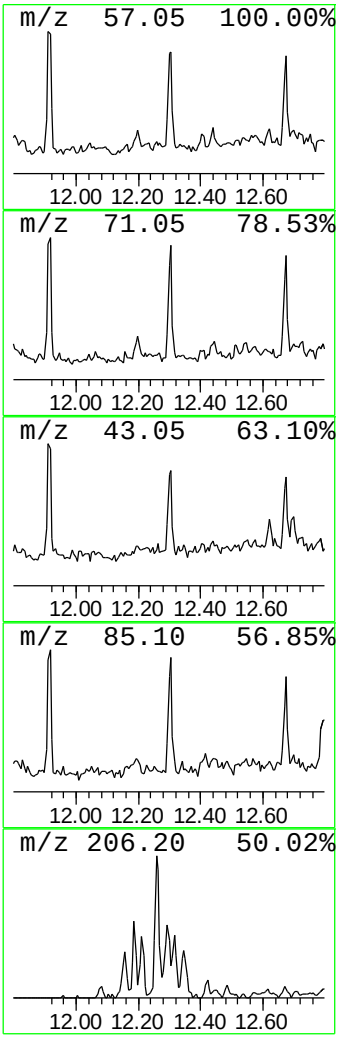
Peak Number 10 unknown12.30 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.30	2.29 ng	82576	Phenanthrene-d10	11.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, hexyl pentyl ester	236	C11H24O3S	1000309-14-1	43
2	Heptacosane	380	C27H56	000593-49-7	43
3	Heptadecane	240	C17H36	000629-78-7	43
4	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	43
5	Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	38





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Instrument : BNA_F
ClientSampleId : G55A-2.5-4.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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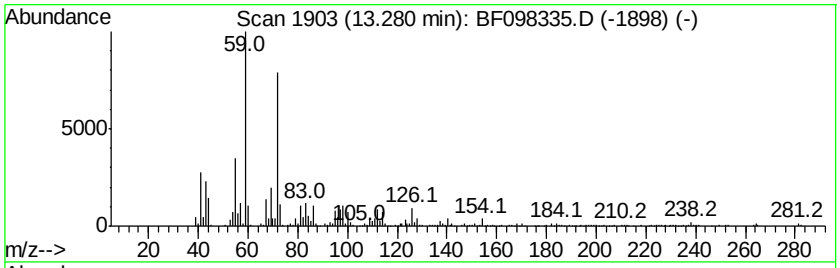
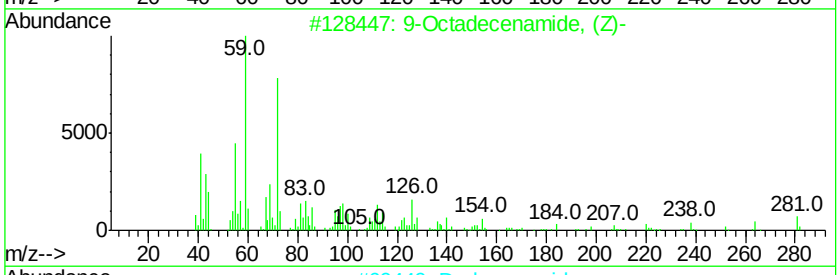
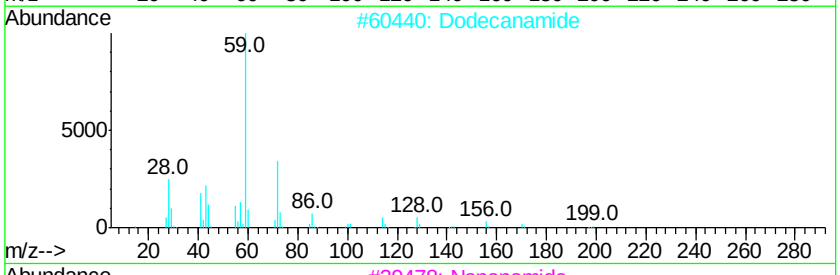
Peak Number 11 9-Octadecenamide, (Z)- Concentration Rank 3

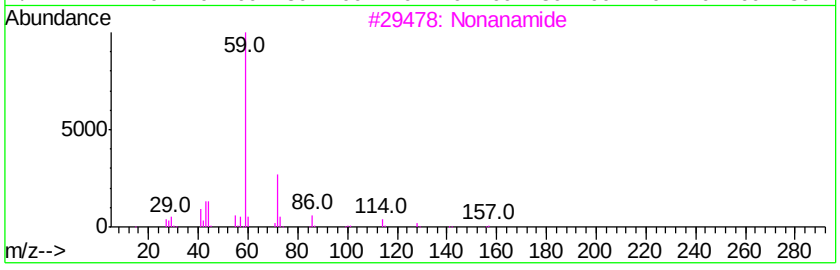
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.28	10.73 ng	522080	Chrysene-d12	13.85

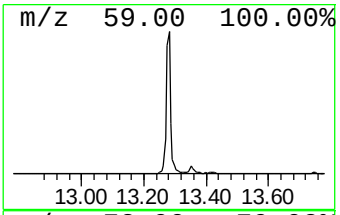
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	98
2	Dodecanamide	199	C12H25NO	001120-16-7	47
3	Nonanamide	157	C9H19NO	001120-07-6	47
4	Undecanamide, 11-bromo-	263	C11H22BrNO	005875-26-3	47
5	Hexadecanamide	255	C16H33NO	000629-54-9	47

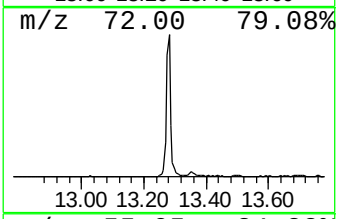


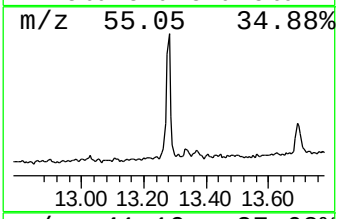


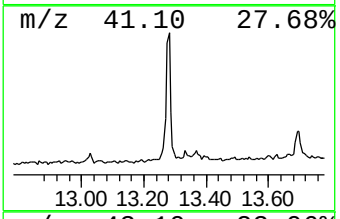


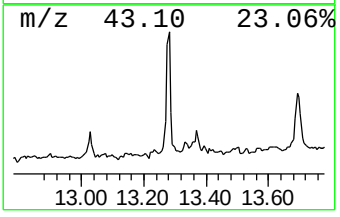












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Instrument : BNA_F
ClientSampleId : G55A-2.5-4.5

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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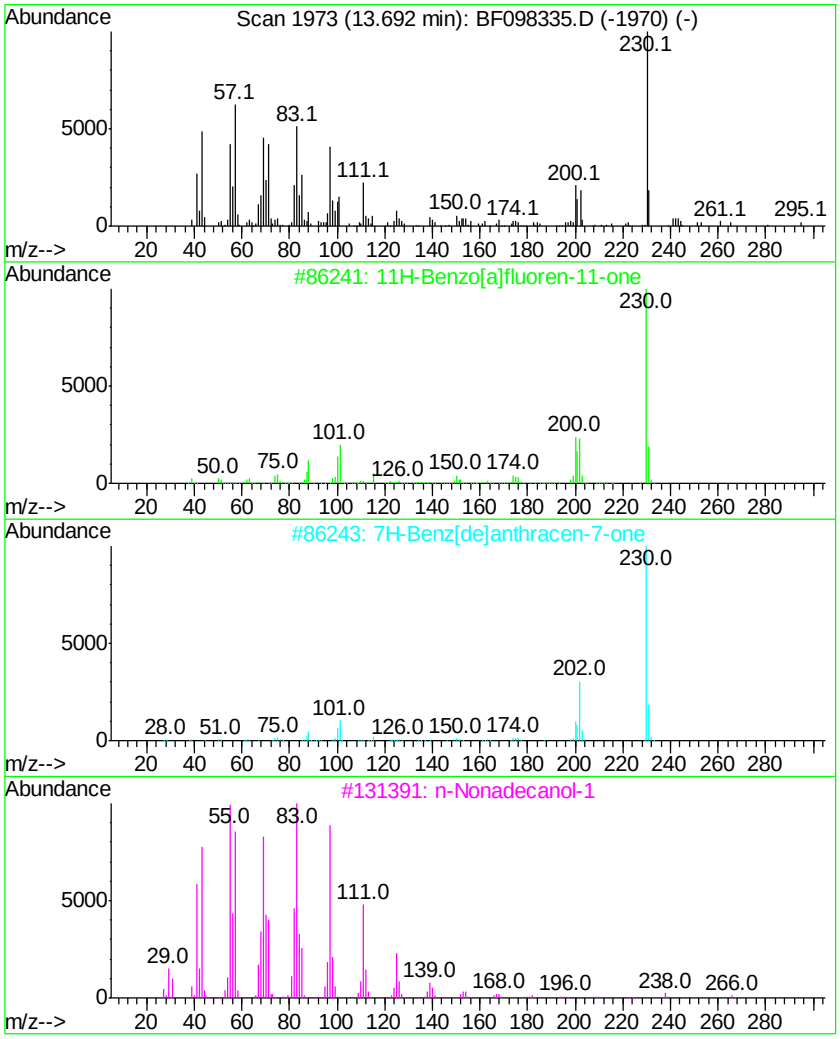
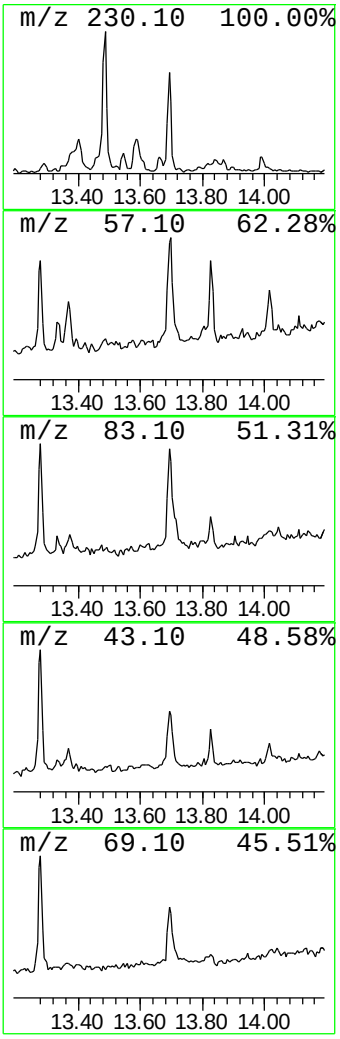
Peak Number 12 unknown13.69 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.69	3.36 ng	163591	Chrysene-d12	13.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[a]fluoren-11-one	230	C17H10O	000479-79-8	41
2	7H-Benz[de]anthracen-7-one	230	C17H10O	000082-05-3	38
3	n-Nonadecanol-1	284	C19H40O	001454-84-8	38
4	1-Dodecanol, 2-hexyl-	270	C18H38O	110225-00-8	38
5	1-Decanol, 2-octyl-	270	C18H38O	045235-48-1	30





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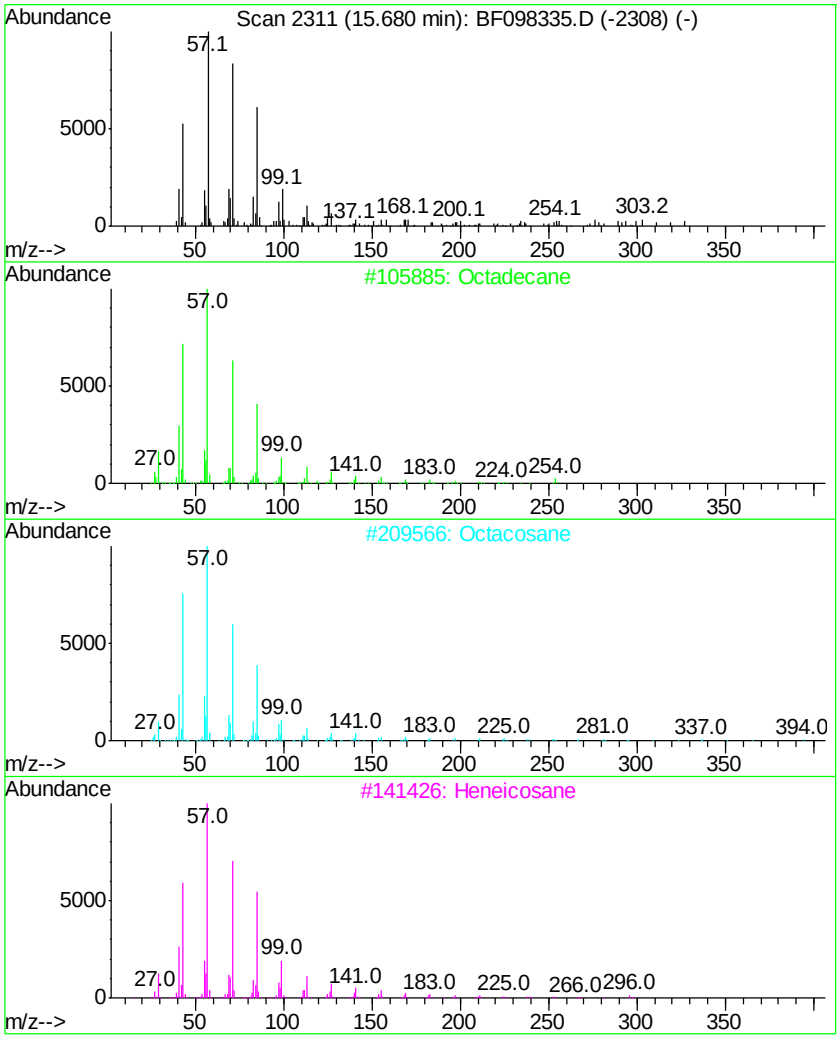
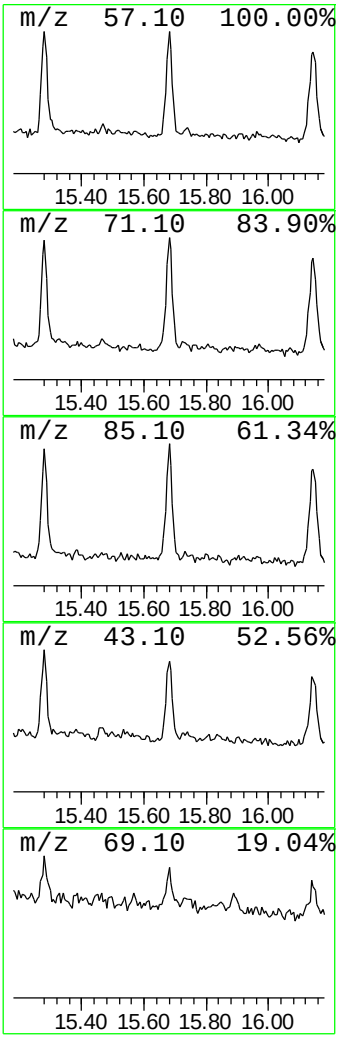
Peak Number 14 Octadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.68	4.11 ng	112091	Perylene-d12	15.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	87
2	Octacosane	394	C28H58	000630-02-4	87
3	Heneicosane	296	C21H44	000629-94-7	87
4	Hexacosane	366	C26H54	000630-01-3	87
5	6,6-Diethylhexadecane	282	C20H42	1000360-41-4	86





Tentatively Identified Compound (LSC) summary

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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...	4.88	7.9	ng	271190	1	6.69	686418	20.0
unknown6.46	6.46	79.9	ng	2741340	1	6.69	686418	20.0
Tridecane	10.63	4.7	ng	167782	4	11.21	721419	20.0
Dodecane, 1-iodo-	11.08	2.3	ng	82253	4	11.21	721419	20.0
Phenanthrene, 2-m...	11.74	2.1	ng	76736	4	11.21	721419	20.0
Phenanthrene, 1-m...	11.82	2.5	ng	89969	4	11.21	721419	20.0
unknown12.30	12.30	2.3	ng	82576	4	11.21	721419	20.0
9-Octadecenamide,...	13.28	10.7	ng	522080	5	13.85	973200	20.0
unknown13.69	13.69	3.4	ng	163591	5	13.85	973200	20.0
Octadecane	15.68	4.1	ng	112091	6	15.26	545936	20.0