LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092217\
Data File : BF098691.D
Acq On : 22 Sep 2017 11:11
Operator : SJ/JU
Sample : I5293-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1-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-BF092117.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	2.263	26	30	52	rVB2	99590	224728	6.04%	0.575%
2	5.163	519	523	536	rBV	502234	655159	17.60%	1.676%
3	5.551	583	589	592	rBV	3419988	3678313	98.80%	9.409%
4	6.545	752	758	763	rBV	3140864	3723007	100.00%	9.523%
5	6.698	779	784	787	rBV	3671352	3721971	99.97%	9.521%
6	6.928	819	823	826	rVB	1136592	908208	24.39%	2.323%
7	7.081	845	849	853	rBV	2743502	2600772	69.86%	6.653%
8	7.487	913	918	921	rBV	2308998	2229793	59.89%	5.704%
9	8.210	1034	1041	1043	rBV	1237162	1194886	32.09%	3.057%
10	8.228	1043	1044	1047	rVB	73047	39949	1.07%	0.102%
11	9.281	1218	1223	1226	rBV	3674734	3201458	85.99%	8.189%
12	9.357	1232	1236	1238	rBV3	50632	49939	1.34%	0.128%
13	9.669	1286	1289	1293	rVB	414066	327057	8.78%	0.837%
14	9.822	1312	1315	1318	rBV	45786	45019	1.21%	0.115%
15	9.886	1321	1326	1328	rVB2	34068	44277	1.19%	0.113%
16	9.963	1333	1339	1342	rBV	1247291	1095666	29.43%	2.803%
17	9.992	1342	1344	1347	rVB	168250	129446	3.48%	0.331%
18	10.163	1368	1373	1377	rVB2	92830	96028	2.58%	0.246%
19	10.204	1377	1380	1385	rVB4	36354	40214	1.08%	0.103%
20	10.275	1388	1392	1395	rBV2	41704	43348	1.16%	0.111%
21	10.369	1404	1408	1409	rBV3	32141	42292	1.14%	0.108%
22	10.386	1409	1411	1414	rVB	70719	52989	1.42%	0.136%
23	10.504	1428	1431	1437	rVB	128204	131239	3.53%	0.336%
24	10.575	1437	1443	1444	rBV3	33626	46488	1.25%	0.119%
25	10.598	1444	1447	1453	rVV2	209012	240564	6.46%	0.615%
26	10.663	1456	1458	1465	rVV	53968	60281	1.62%	0.154%
27	10.751	1467	1473	1476	rVV	1869764	1798539	48.31%	4.601%
28	10.792	1476	1480	1484	rVV	234464	237897	6.39%	0.609%
29	10.869	1488	1493	1499	rVB2	98597	158954	4.27%	0.407%
30	11.022	1515	1519	1521	rBV	56929	56687	1.52%	0.145%
31	11.051	1521	1524	1527	rVB3	50857	59261	1.59%	0.152%
32	11.304	1562	1567	1570	rBV3	63897	79929	2.15%	0.204%
33	11.345	1570	1574	1579	rVB2	77854	98017	2.63%	0.251%
34	11.451	1588	1592	1594	rBV	932994	974666	26.18%	2.493%

LSC Area Percent Report

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Operator : SJ/JU
Sample : I5293-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1-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-BF092117.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	11.475	1594	1596	1599	rVV	754999	599873	16.11%	1.534%
36	11.522	1601	1604	1607	rVB	378599	282664	7.59%	0.723%
37	11.675	1628	1630	1637	rVB	49570	47284	1.27%	0.121%
38	11.951	1674	1677	1678	rBV	108337	116537	3.13%	0.298%
39	11.975	1678	1681	1684	rVV2	185779	229258	6.16%	0.586%
40	12.022	1686	1689	1692	rVV	62305	63294	1.70%	0.162%
41	12.063	1692	1696	1698	rVV	297526	301558	8.10%	0.771%
42	12.080	1698	1699	1702	rVB	97066	65102	1.75%	0.167%
43	12.245	1724	1727	1729	rBV	112470	106060	2.85%	0.271%
44	12.498	1766	1770	1772	rBV	79052	87082	2.34%	0.223%
45	12.527	1772	1775	1778	rVV4	45089	63003	1.69%	0.161%
46	12.580	1782	1784	1789	rBV3	38225	48483	1.30%	0.124%
47	12.663	1794	1798	1801	rBV	1481915	1287518	34.58%	3.293%
48	12.751	1810	1813	1816	rBV3	117855	125814	3.38%	0.322%
49	12.810	1821	1823	1826	rVV	72113	83427	2.24%	0.213%
50	12.892	1830	1837	1842	rVV	1137989	1253185	33.66%	3.206%
51	12.933	1842	1844	1849	rVB2	45111	63278	1.70%	0.162%
52	13.004	1854	1856	1857	rBV	52525	43180	1.16%	0.110%
53	13.033	1857	1861	1864	rVB	2611112	2306711	61.96%	5.901%
54	13.098	1869	1872	1876	rBV4	55374	96788	2.60%	0.248%
55	13.216	1889	1892	1896	rVB2	147267	133430	3.58%	0.341%
56	13.280	1900	1903	1906	rBV	123636	103056	2.77%	0.264%
57	13.316	1907	1909	1912	rVB2	62805	61124	1.64%	0.156%
58	13.439	1928	1930	1933	rBV	41745	45039	1.21%	0.115%
59	13.863	2000	2002	2004	rBV	56702	42998	1.15%	0.110%
60	13.916	2009	2011	2016	rVB2	226959	214173	5.75%	0.548%
61	14.086	2033	2040	2042	rBV2	1121465	1370843	36.82%	3.507%
62	14.110	2042	2044	2050	rVB	346746	294462	7.91%	0.753%
63	15.133	2215	2218	2222	rBV	213825	342382	9.20%	0.876%
64	15.510	2279	2282	2286	rBV	167512	183919	4.94%	0.470%
65	15.580	2289	2294	2298	rBV	722546	944565	25.37%	2.416%

Sum of corrected areas: 39093131

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Misc :
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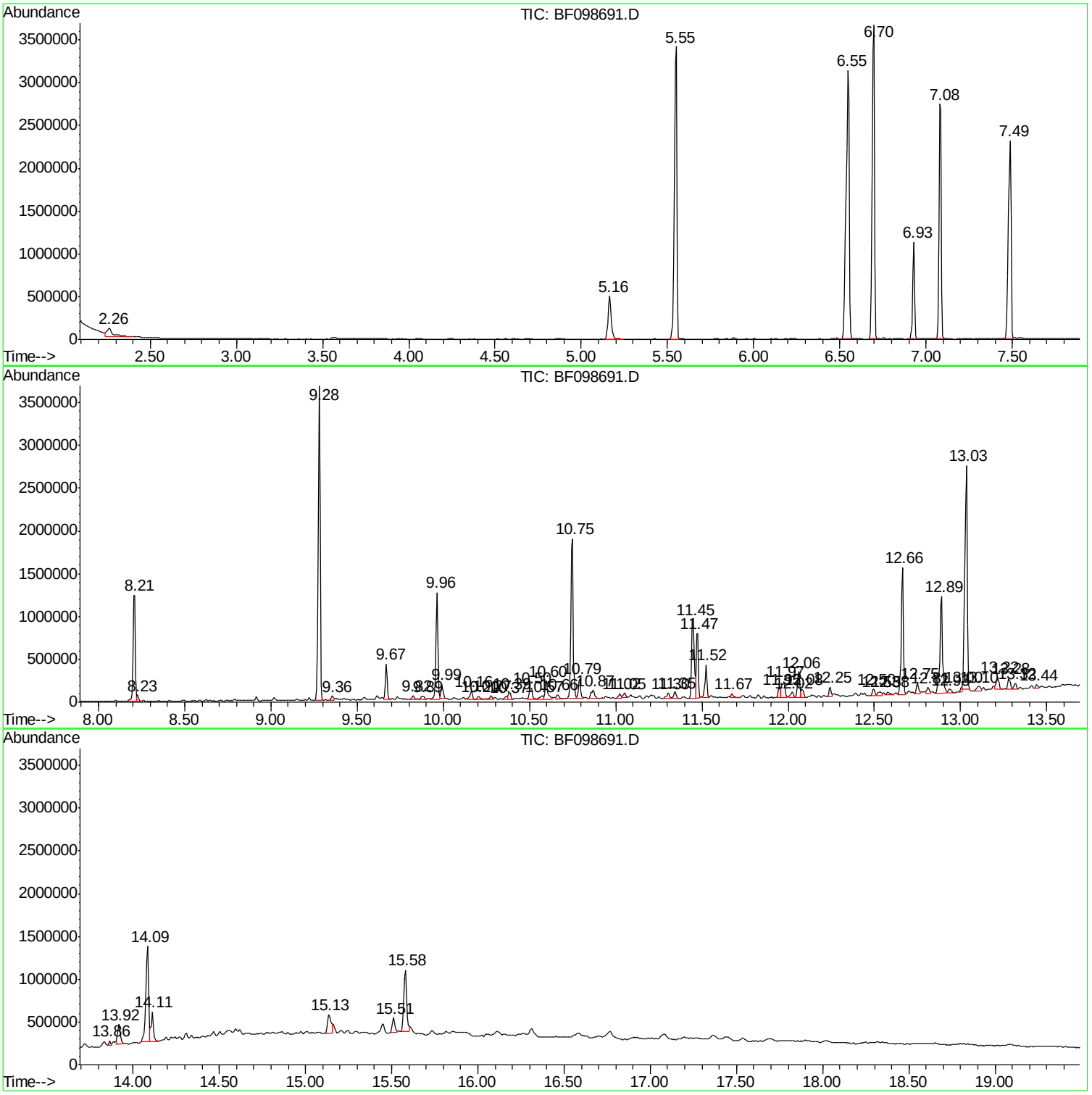
Instrument :
BNA_F
ClientSampleId :
TP-1-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

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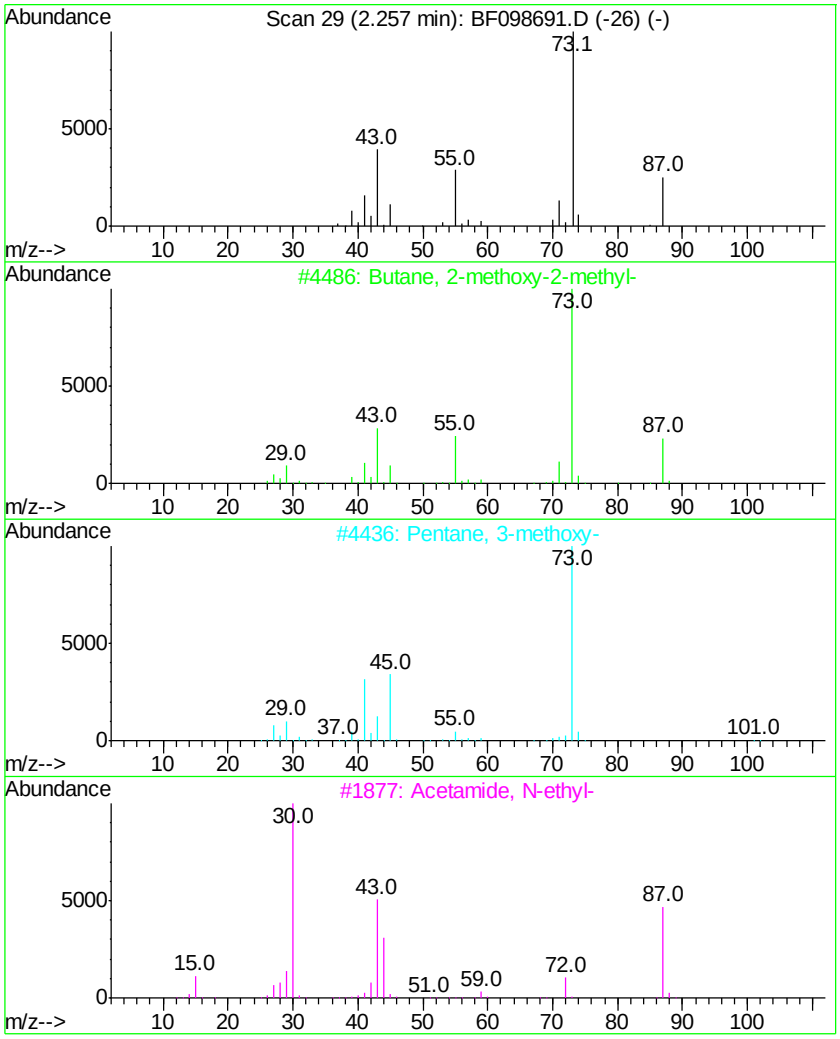
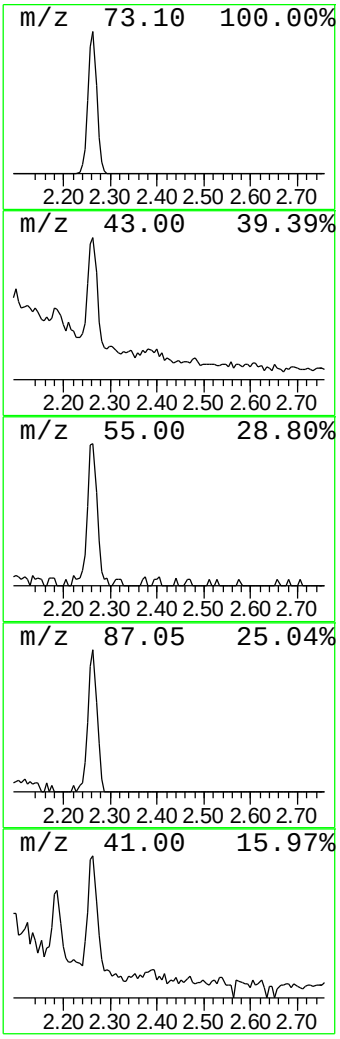
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.26	4.95 ng	224728	1,4-Dichlorobenzene-d4	6.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
3	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
4	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	Boronic acid, ethyl-, dimethyl e...	102	C4H11BO2	007318-82-3	9





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Misc :
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Instrument : BNA_F
ClientSampleId : TP-1-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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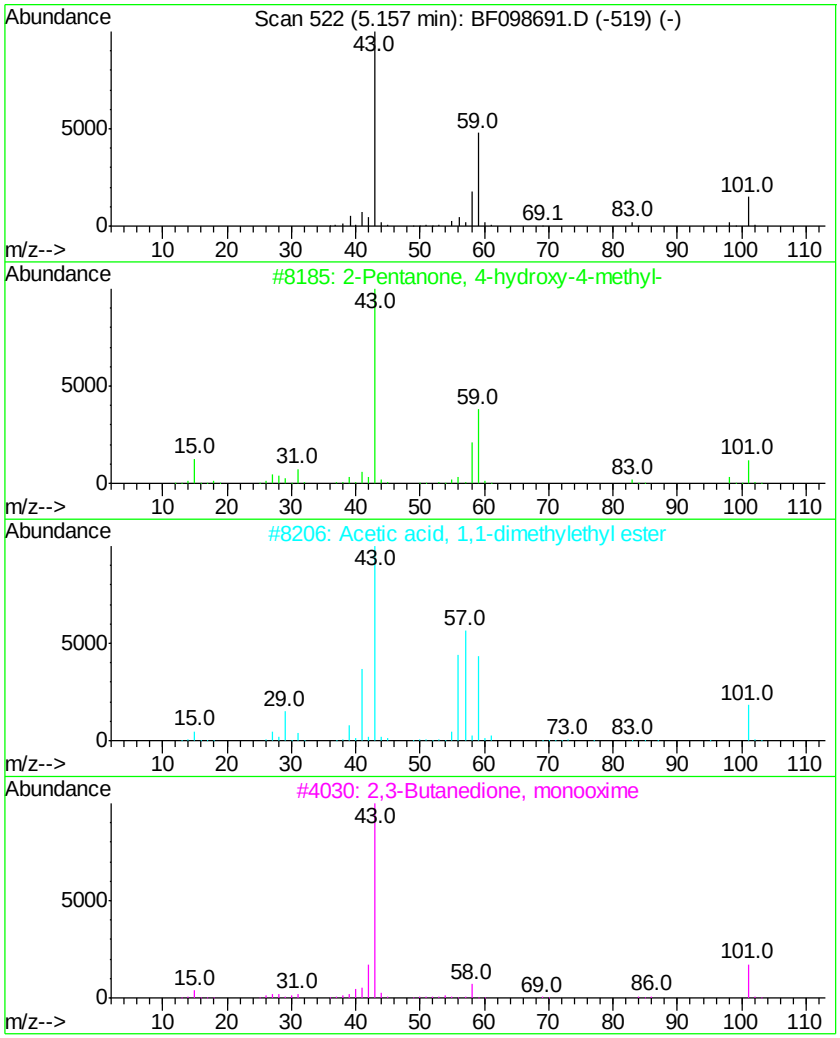
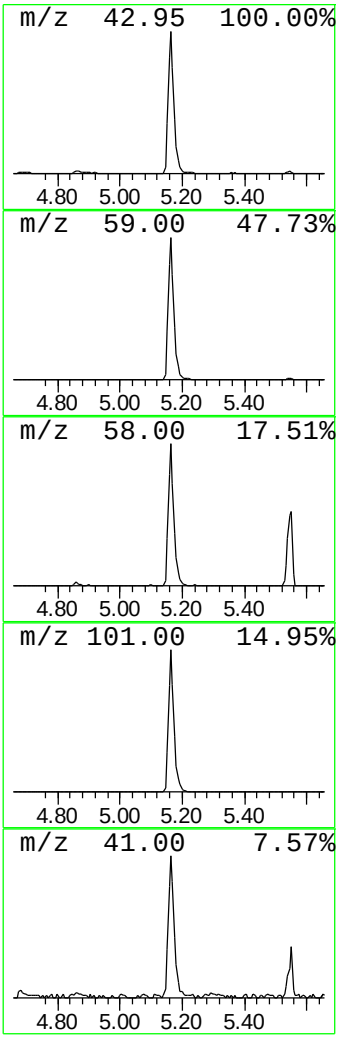
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.16	14.43 ng	655159	1,4-Dichlorobenzene-d4	6.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	Acetone	58	C3H6O	000067-64-1	9





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Instrument : BNA_F
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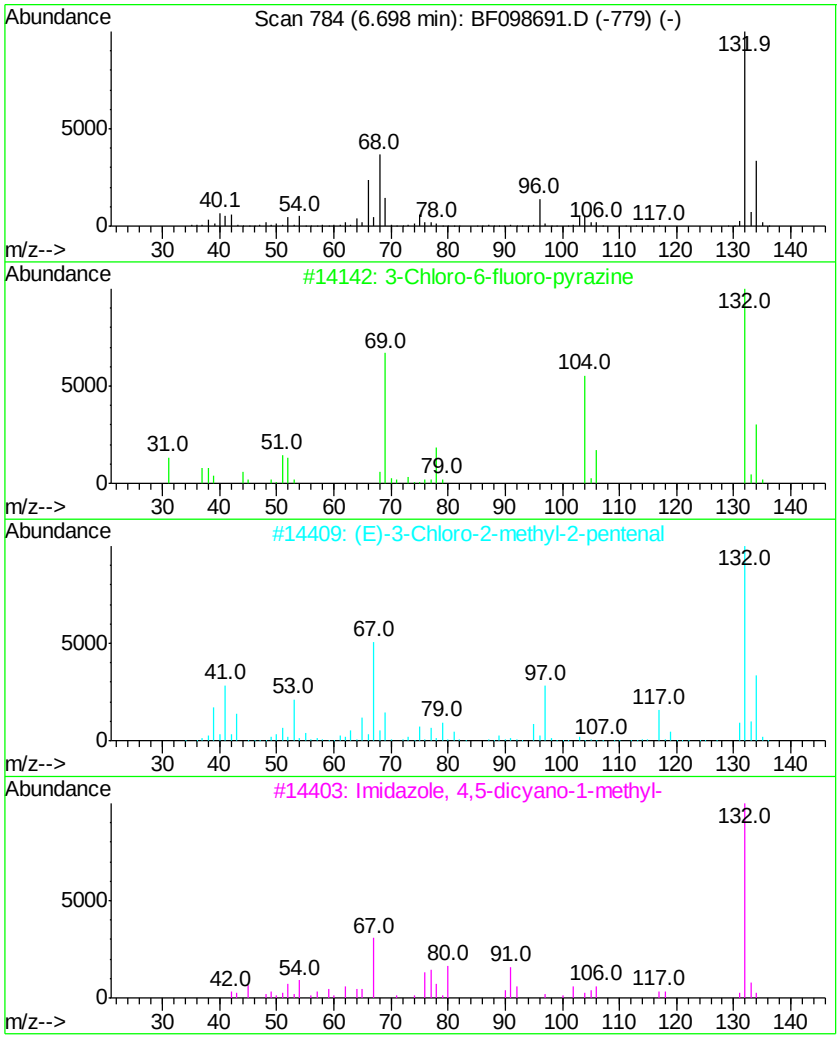
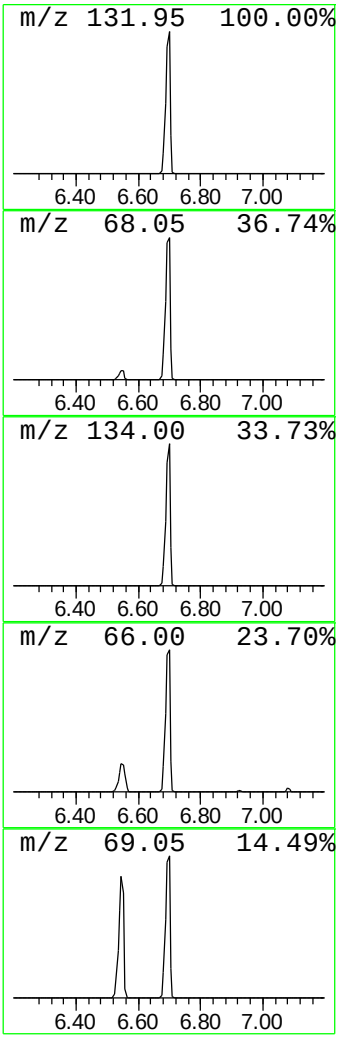
Peak Number 3 unknown6.70 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.70	81.96 ng	3721970	1,4-Dichlorobenzene-d4	6.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9
4	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





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Instrument : BNA_F
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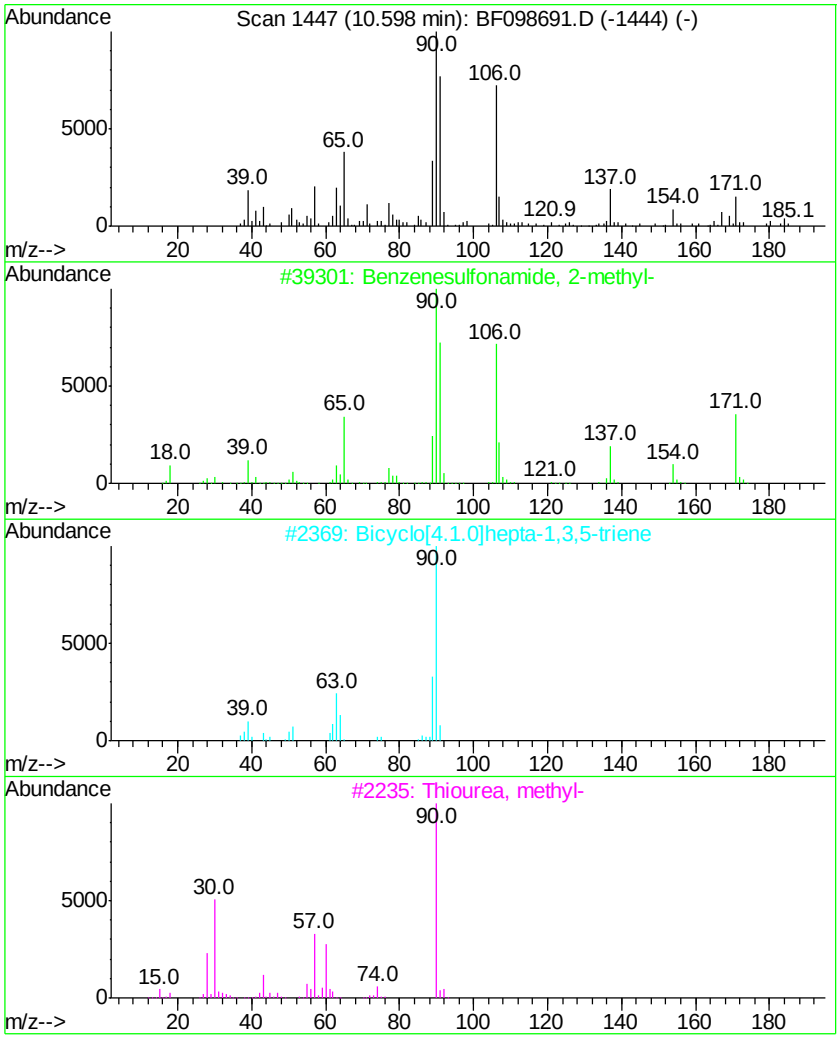
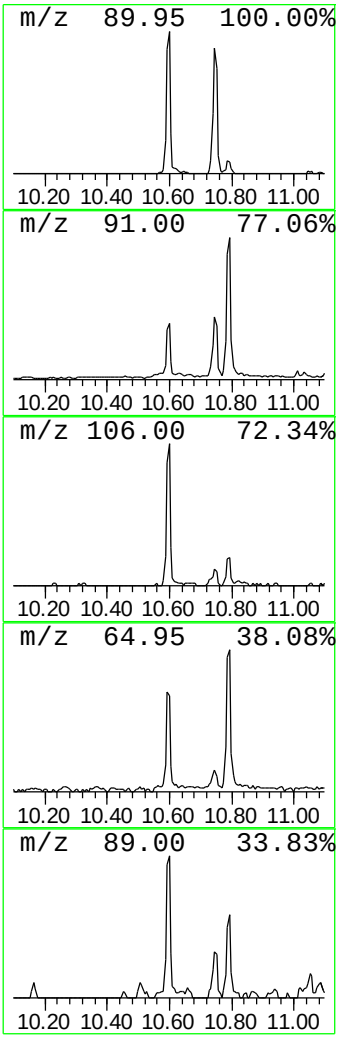
Peak Number 5 Benzenesulfonamide, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.60	4.39 ng	240564	Acenaphthene-d10	9.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenesulfonamide, 2-methyl-	171	C7H9NO2S	000088-19-7	94
2	Bicyclo[4.1.0]hepta-1,3,5-triene	90	C7H6	004646-69-9	43
3	Thiourea, methyl-	90	C2H6N2S	000598-52-7	32
4	4-(2-Aminoethyl)benzenesulfonamide	200	C8H12N2O2S	035303-76-5	28
5	2,4-Octadiyne	106	C8H10	002809-71-4	25





Library Search Compound Report

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Instrument : BNA_F
ClientSampleId : TP-1-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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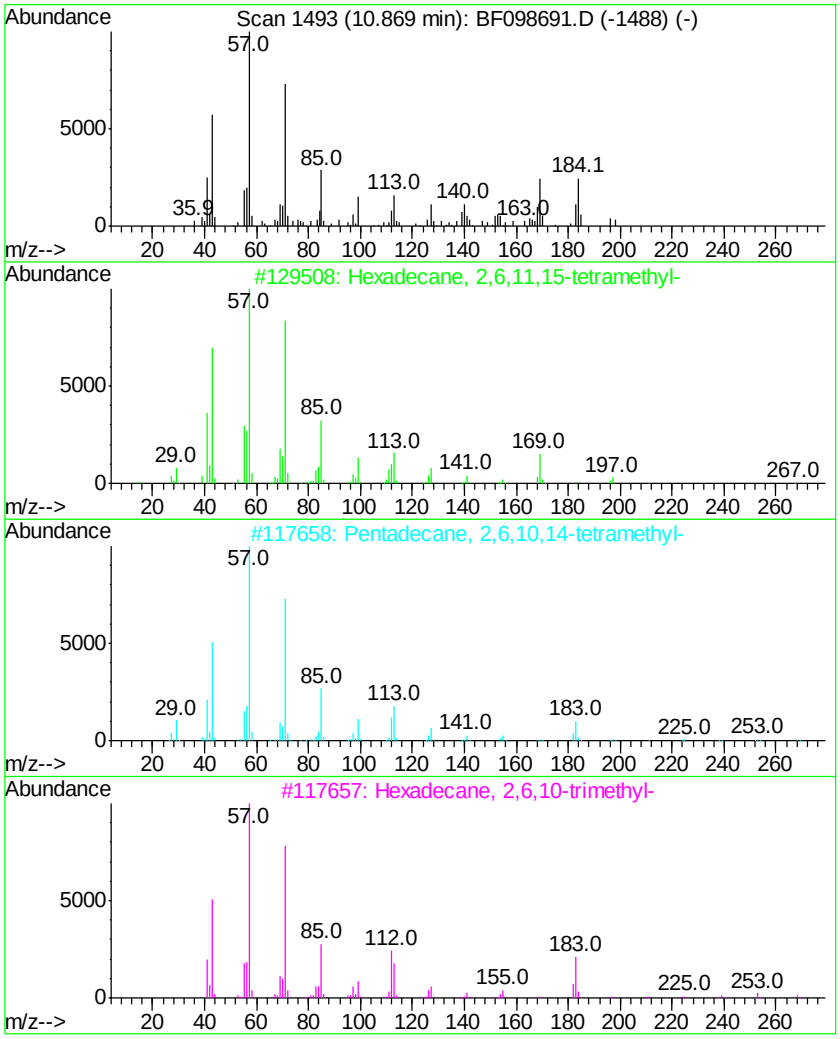
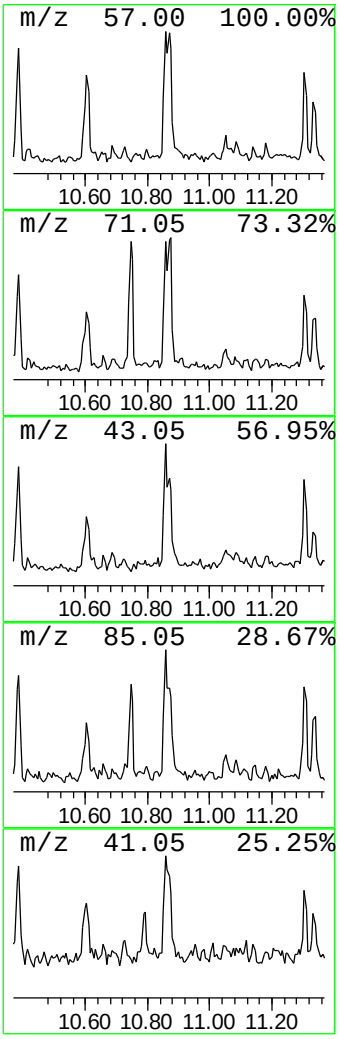
****

Peak Number 6 Hexadecane, 2,6,11,15-tetra... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.87	3.26 ng	158954	Phenanthrene-d10	11.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane, 2,6,11,15-tetramethyl-	282	C20H42	000504-44-9	58
2	Pentadecane, 2,6,10,14-tetramethyl-	268	C19H40	001921-70-6	52
3	Hexadecane, 2,6,10-trimethyl-	268	C19H40	055000-52-7	49
4	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	49
5	Decane, 5-ethyl-5-methyl-	184	C13H28	017312-74-2	46





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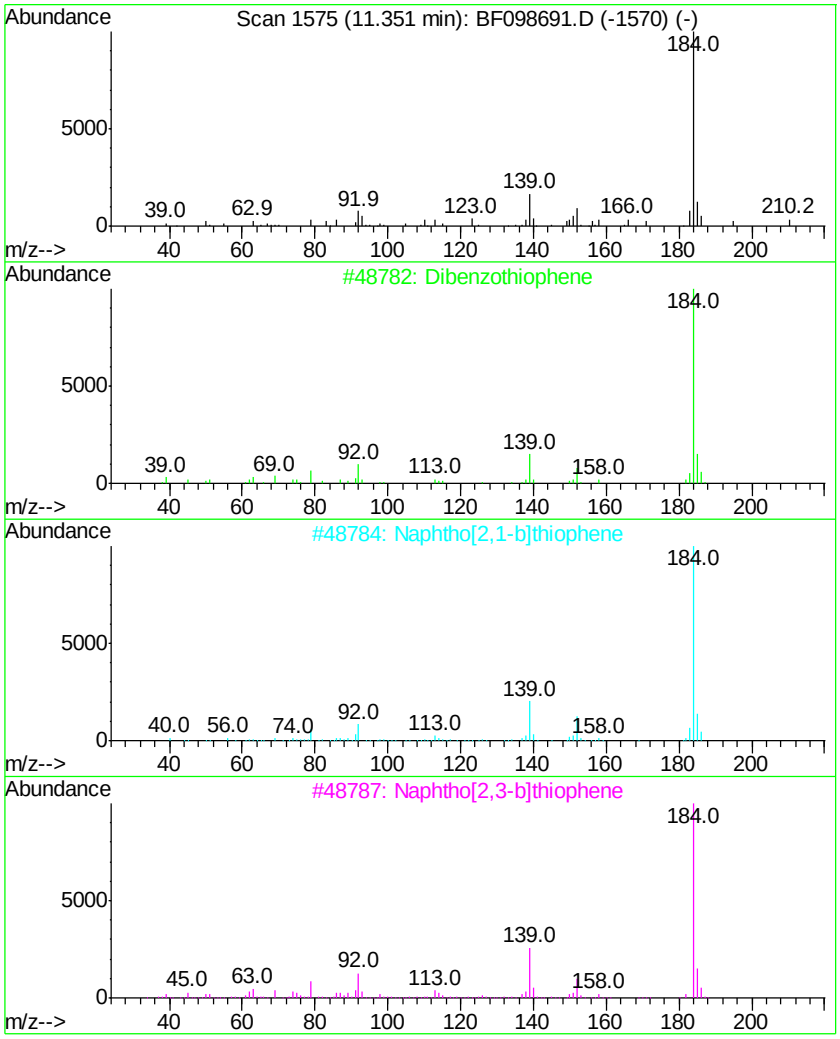
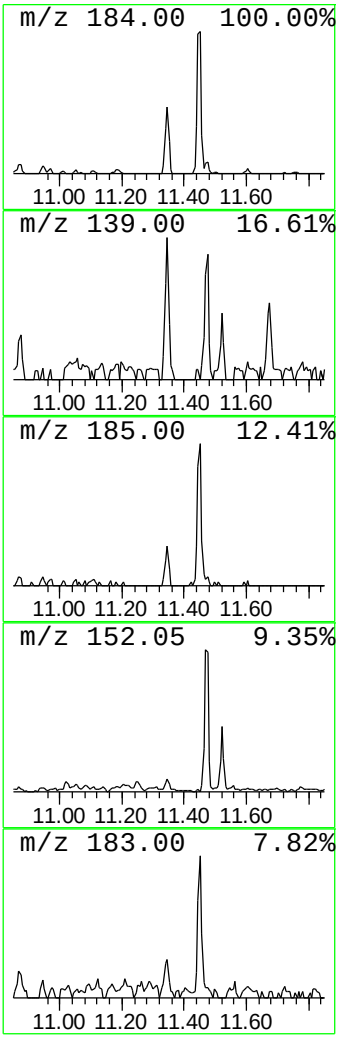
****

Peak Number 7 Dibenzothiophene Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.35	2.01 ng	98017	Phenanthrene-d10	11.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dibenzothiophene	184	C12H8S	000132-65-0	96
2	Naphtho[2,1-b]thiophene	184	C12H8S	000233-02-3	94
3	Naphtho[2,3-b]thiophene	184	C12H8S	000268-77-9	93
4	Naphtho[1,2-b]thiophene	184	C12H8S	000234-41-3	93
5	Azuleno(2,1-b)thiophene	184	C12H8S	000248-13-5	91





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Sample : I5293-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092117.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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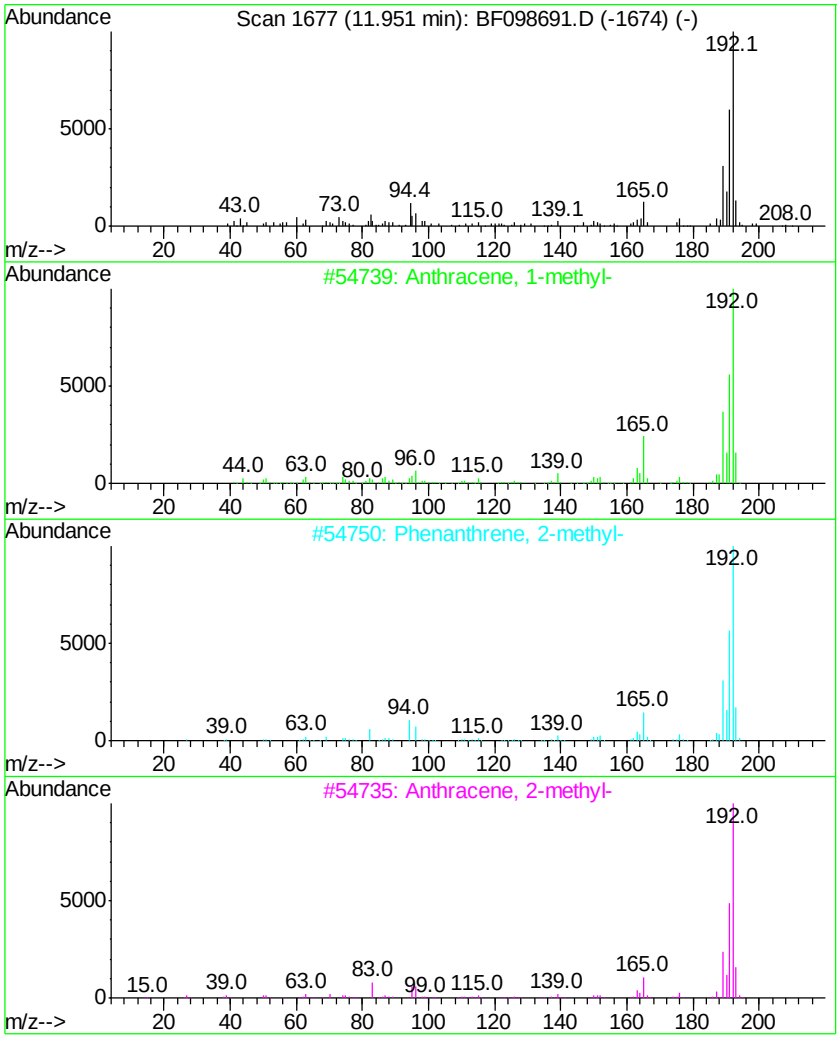
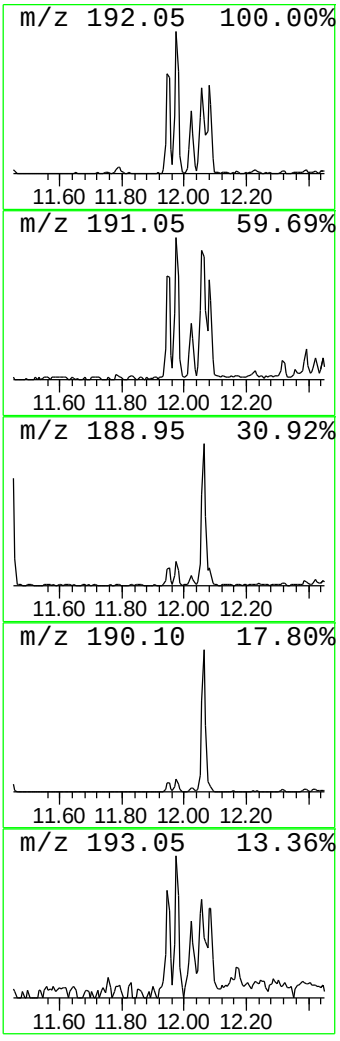
Peak Number 8 Anthracene, 1-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.95	2.39 ng	116537	Phenanthrene-d10	11.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 1-methyl-	192	C15H12	000610-48-0	93
2	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	93
3	Anthracene, 2-methyl-	192	C15H12	000613-12-7	91
4	Anthracene, 9-methyl-	192	C15H12	000779-02-2	90
5	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	89





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Data File : BF098691.D
Acq On : 22 Sep 2017 11:11
Operator : SJ/JU
Sample : I5293-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

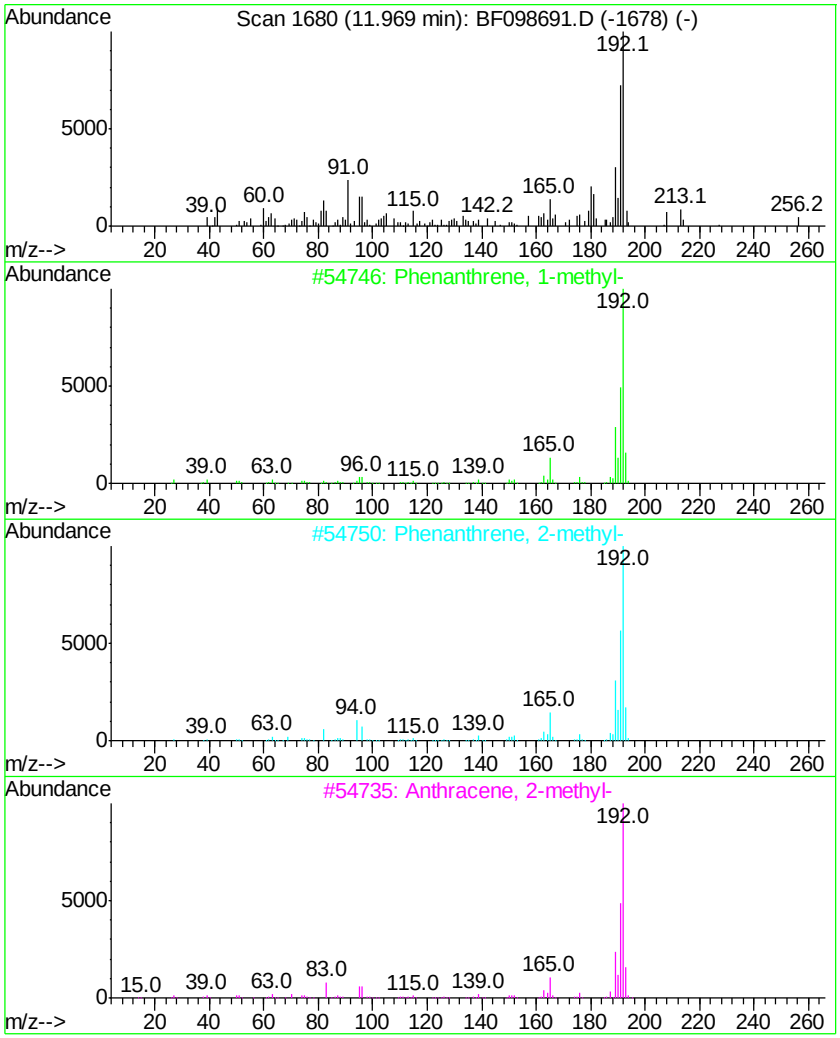
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

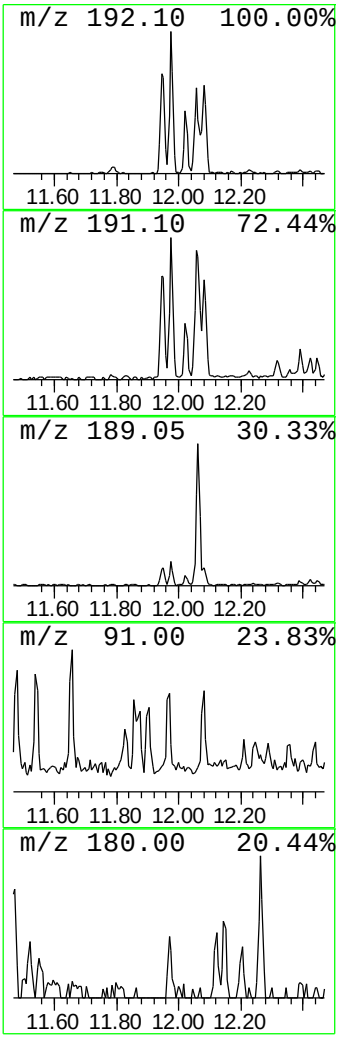
****

Peak Number 9 Phenanthrene, 1-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.97	4.70 ng	229258	Phenanthrene-d10	11.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	96
2	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	96
3	Anthracene, 2-methyl-	192	C15H12	000613-12-7	96
4	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	94
5	Anthracene, 1-methyl-	192	C15H12	000610-48-0	91





Data Path : Z:\HPCHEM1\BNA F\DATA\BF092217\
Data File : BF098691.D
Acq On : 22 Sep 2017 11:11
Operator : SJ/JU
Sample : I5293-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092117.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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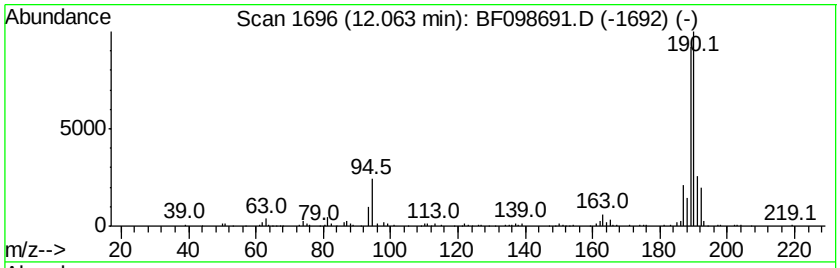
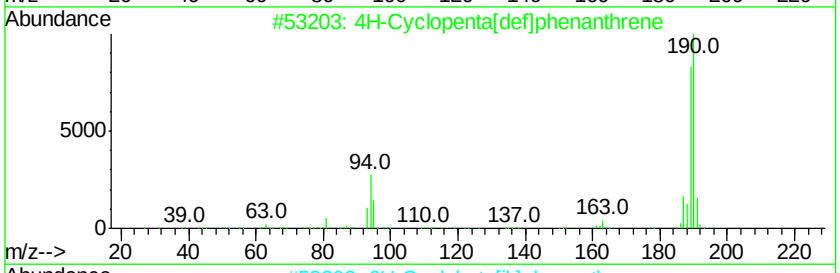
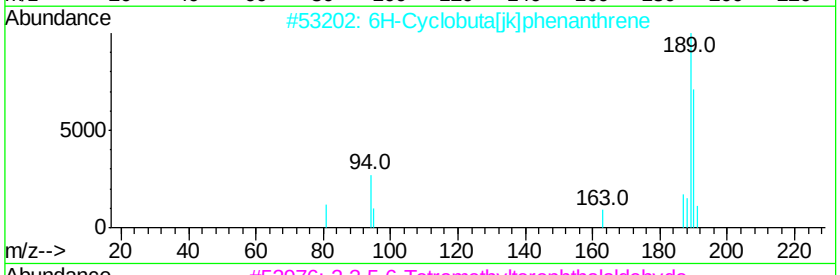
Peak Number 10 4H-Cyclopenta[def]phenanthrene Concentration Rank 4

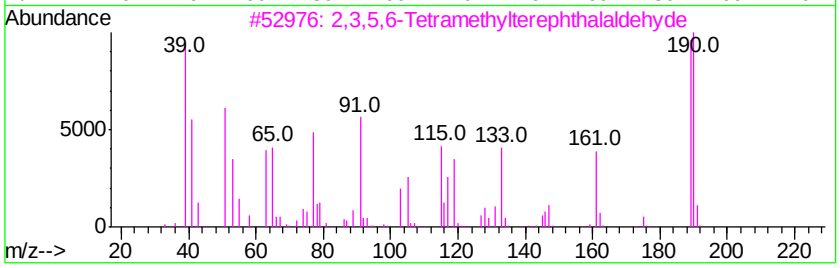
R.T.	EstConc	Area	Relative to ISTD	R.T.
12.06	6.19 ng	301558	Phenanthrene-d10	11.45

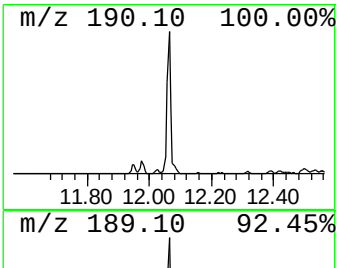
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	94
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	50
3	2,3,5,6-Tetramethylterephthalald...	190	C12H14O2	007072-01-7	47
4	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	42
5	Hydrazinecarboxaldehyde, 2-[3-(m...	190	C4H6N4OS2	038362-25-3	14

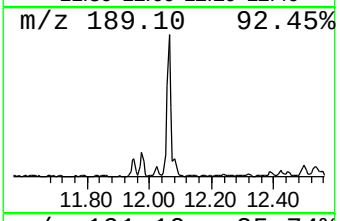


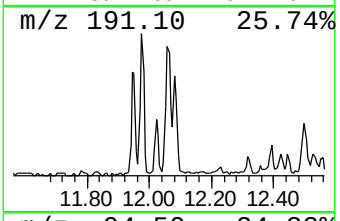


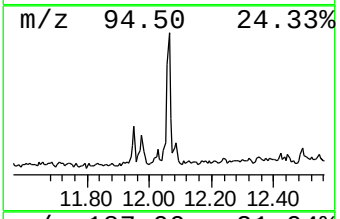


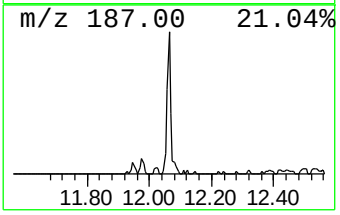












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ClientSampleId : TP-1-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092117.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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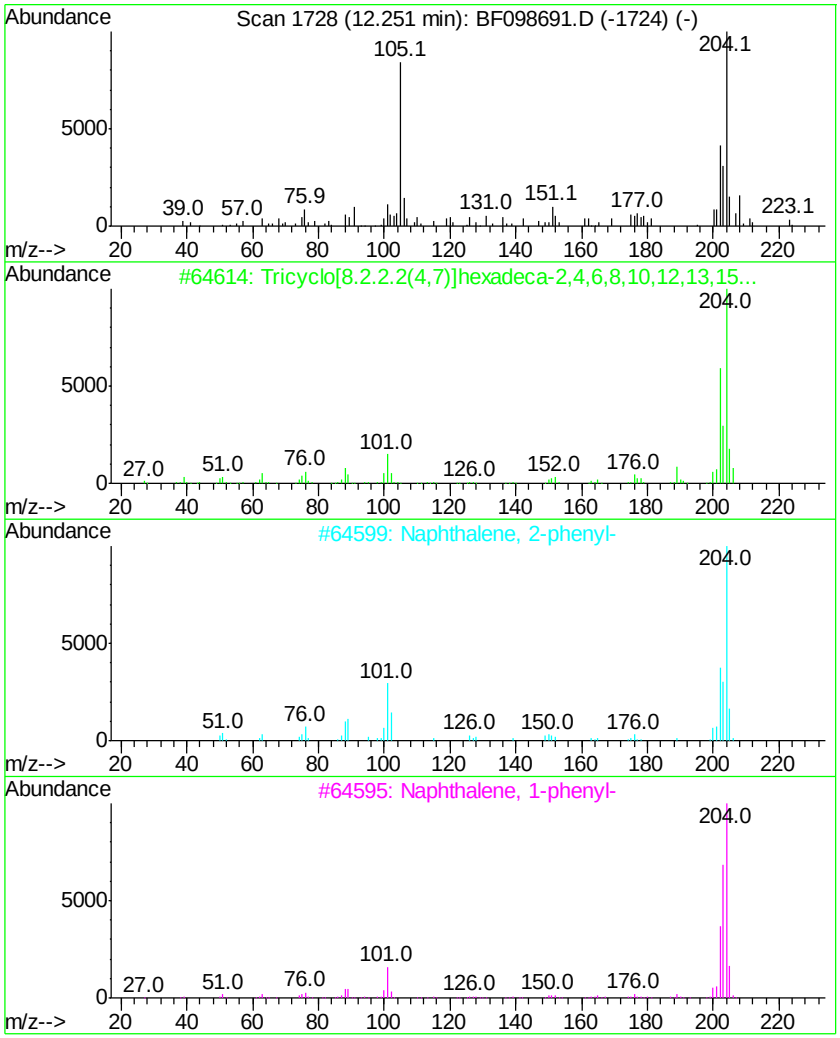
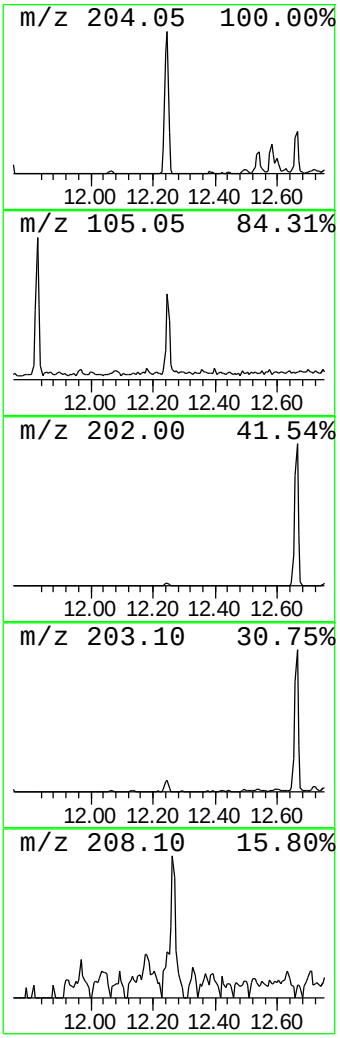
Peak Number 11 Tricyclo[8.2.2.2(4,7)]hexad... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.25	2.18 ng	106060	Phenanthrene-d10	11.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tricyclo[8.2.2.2(4,7)]hexadeca-2...	204	C16H12	006572-60-7	64
2	Naphthalene, 2-phenyl-	204	C16H12	000612-94-2	60
3	Naphthalene, 1-phenyl-	204	C16H12	000605-02-7	55
4	9,10-Bis(bromomethyl)anthracene	362	C16H12Br2	034373-96-1	52
5	6-Cyanophenanthridine	204	C14H8N2	002176-28-5	45





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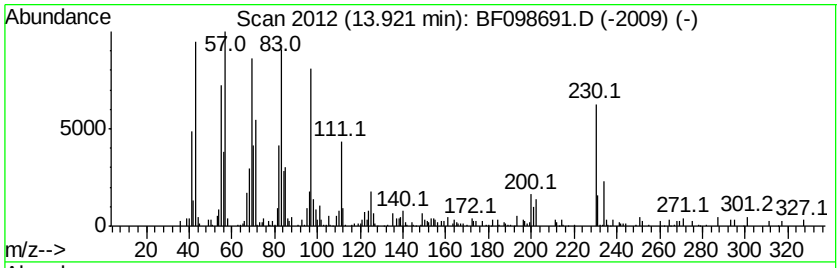
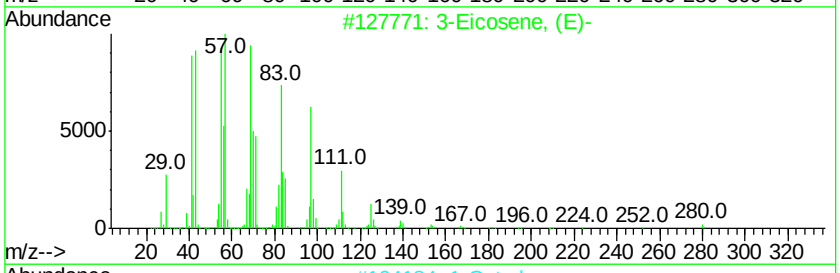
****

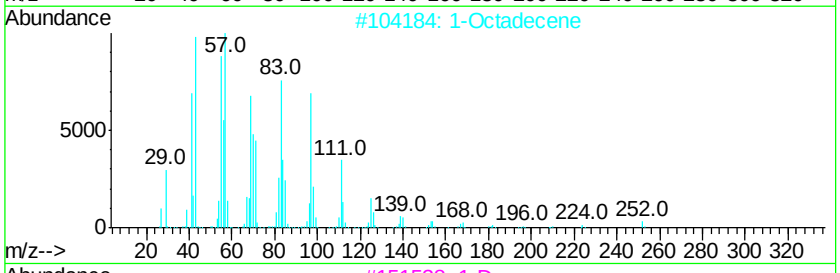
Peak Number 13 3-Eicosene, (E)- Concentration Rank 9

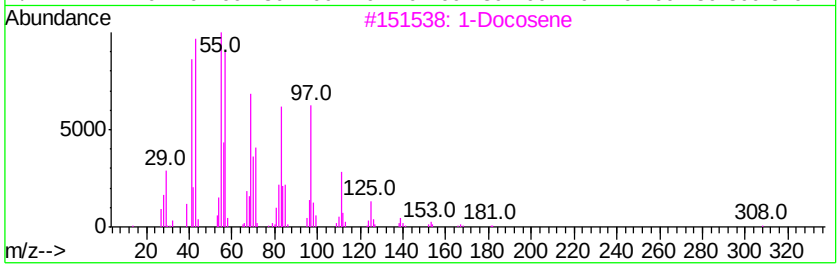
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.92	3.12 ng	214173	Chrysene-d12	14.09

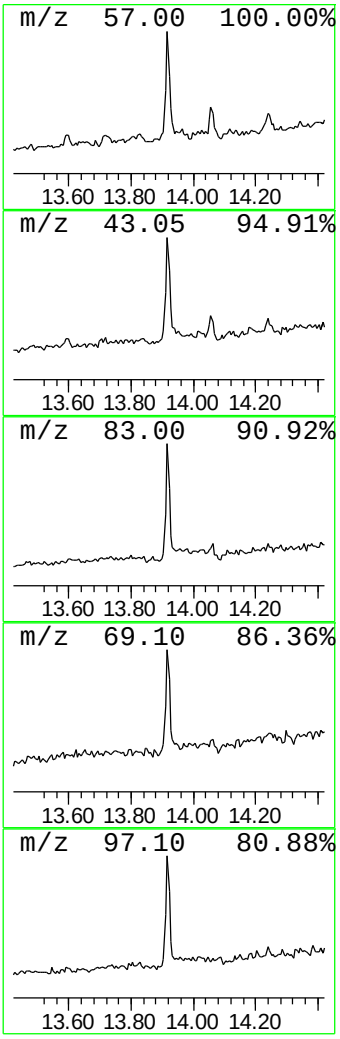
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-	280	C20H40	074685-33-9	97
2	1-Octadecene	252	C18H36	000112-88-9	93
3	1-Docosene	308	C22H44	001599-67-3	93
4	Behenic alcohol	326	C22H46O	000661-19-8	93
5	1-Heneicosanol	312	C21H44O	015594-90-8	90











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
Butane, 2-methoxy...	2.26	5.0	ng	224728	1	6.93	908208	20.0
2-Pentanone, 4-hy...	5.16	14.4	ng	655159	1	6.93	908208	20.0
unknown6.70	6.70	82.0	ng	3721970	1	6.93	908208	20.0
Benzenesulfonamid...	10.60	4.4	ng	240564	3	9.96	1095670	20.0
Hexadecane, 2,6,1...	10.87	3.3	ng	158954	4	11.45	974666	20.0
Dibenzothiophene	11.35	2.0	ng	98017	4	11.45	974666	20.0
Anthracene, 1-met...	11.95	2.4	ng	116537	4	11.45	974666	20.0
Phenanthrene, 1-m...	11.97	4.7	ng	229258	4	11.45	974666	20.0
4H-Cyclopenta[def...	12.06	6.2	ng	301558	4	11.45	974666	20.0
Tricyclo[8.2.2.2(...	12.25	2.2	ng	106060	4	11.45	974666	20.0
3-Eicosene, (E)-	13.92	3.1	ng	214173	5	14.09	1370840	20.0