LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF070517\
Data File : BF096504.D
Acq On : 6 Jul 2017 1:29
Operator : SJ/MA
Sample : I3976-04
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B9-6-8

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-BF070117.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	4.310	372	378	384	rBV2	22091	29596	1.17%	0.114%
2	4.892	472	477	487	rBV	469224	588978	23.25%	2.276%
3	5.322	545	550	553	rBV	2436899	2398567	94.67%	9.268%
4	5.992	661	664	667	rBV	112553	90758	3.58%	0.351%
5	6.351	720	725	728	rBV	2450639	2486357	98.14%	9.607%
6	6.481	743	747	751	rBV	2473216	2430027	95.92%	9.389%
7	6.710	783	786	790	rBV	912117	761386	30.05%	2.942%
8	6.781	795	798	804	rBV3	20451	30076	1.19%	0.116%
9	6.869	809	813	816	rVB	2226688	1900398	75.01%	7.343%
10	7.275	876	882	885	rBV	1602951	1551355	61.23%	5.994%
11	7.375	893	899	904	rBV2	39322	53091	2.10%	0.205%
12	7.992	1000	1004	1007	rBV	1275844	1055247	41.65%	4.077%
13	8.433	1076	1079	1083	rBV2	34632	30572	1.21%	0.118%
14	8.604	1104	1108	1110	rBV	28943	29109	1.15%	0.112%
15	8.704	1121	1125	1128	rVB4	23687	30740	1.21%	0.119%
16	9.075	1183	1188	1191	rBV	2809283	2533481	100.00%	9.789%
17	9.163	1198	1203	1207	rBV3	68635	83391	3.29%	0.322%
18	9.327	1228	1231	1237	rVB6	22111	32526	1.28%	0.126%
19	9.463	1251	1254	1257	rBV	453058	374629	14.79%	1.447%
20	9.692	1291	1293	1297	rVB	81570	71330	2.82%	0.276%
21	9.745	1297	1302	1306	rBV	1014600	955446	37.71%	3.692%
22	9.857	1316	1321	1325	rVB7	13159	30381	1.20%	0.117%
23	9.951	1335	1337	1341	rVB2	43571	39378	1.55%	0.152%
24	10.192	1376	1378	1381	rVB	94180	70994	2.80%	0.274%
25	10.416	1412	1416	1419	rBV	46204	50163	1.98%	0.194%
26	10.533	1432	1436	1440	rBV	1093100	1004378	39.64%	3.881%
27	10.663	1455	1458	1466	rVB2	112152	159889	6.31%	0.618%
28	11.116	1532	1535	1537	rBV2	72533	65077	2.57%	0.251%
29	11.145	1537	1540	1543	rVB	52526	49995	1.97%	0.193%
30	11.227	1550	1554	1556	rBV	870925	754187	29.77%	2.914%
31	11.251	1556	1558	1561	rVB	209602	156242	6.17%	0.604%
32	11.298	1561	1566	1569	rBV	125605	128640	5.08%	0.497%
33	11.463	1590	1594	1597	rBV2	115171	124083	4.90%	0.479%
34	11.539	1605	1607	1612	rVB2	57054	57532	2.27%	0.222%

LSC Area Percent Report

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Misc :
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Instrument : BNA_F
ClientSampleId : B9-6-8

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-BF070117.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	11.639	1621	1624	1629	rBV2	50836	59071	2.33%	0.228%
36	11.727	1637	1639	1641	rBV	40824	28021	1.11%	0.108%
37	11.757	1641	1644	1648	rVB	74044	64433	2.54%	0.249%
38	11.804	1649	1652	1655	rVB2	49742	58738	2.32%	0.227%
39	11.839	1655	1658	1660	rBV	139106	136512	5.39%	0.527%
40	11.863	1660	1662	1664	rVB	48789	37183	1.47%	0.144%
41	12.021	1686	1689	1692	rBV	139172	135273	5.34%	0.523%
42	12.104	1700	1703	1706	rBV4	28040	43000	1.70%	0.166%
43	12.280	1730	1733	1737	rBV2	111258	142368	5.62%	0.550%
44	12.339	1740	1743	1745	rVV	124055	105448	4.16%	0.407%
45	12.439	1756	1760	1763	rBV	792643	698703	27.58%	2.700%
46	12.663	1793	1798	1802	rBV	590845	639994	25.26%	2.473%
47	12.704	1803	1805	1808	rVB2	40937	39291	1.55%	0.152%
48	12.786	1817	1819	1820	rBV	39611	27810	1.10%	0.107%
49	12.815	1820	1824	1827	rVV	1907877	1704507	67.28%	6.586%
50	13.063	1863	1866	1868	rBV2	69762	59190	2.34%	0.229%
51	13.298	1904	1906	1911	rVB	81376	85922	3.39%	0.332%
52	13.721	1976	1978	1984	rVB3	151164	179819	7.10%	0.695%
53	13.862	1997	2002	2004	rBV2	732847	842233	33.24%	3.254%
54	13.886	2004	2006	2009	rVB	179234	134552	5.31%	0.520%
55	15.274	2239	2242	2245	rBV	374246	451113	17.81%	1.743%

Sum of corrected areas: 25881180

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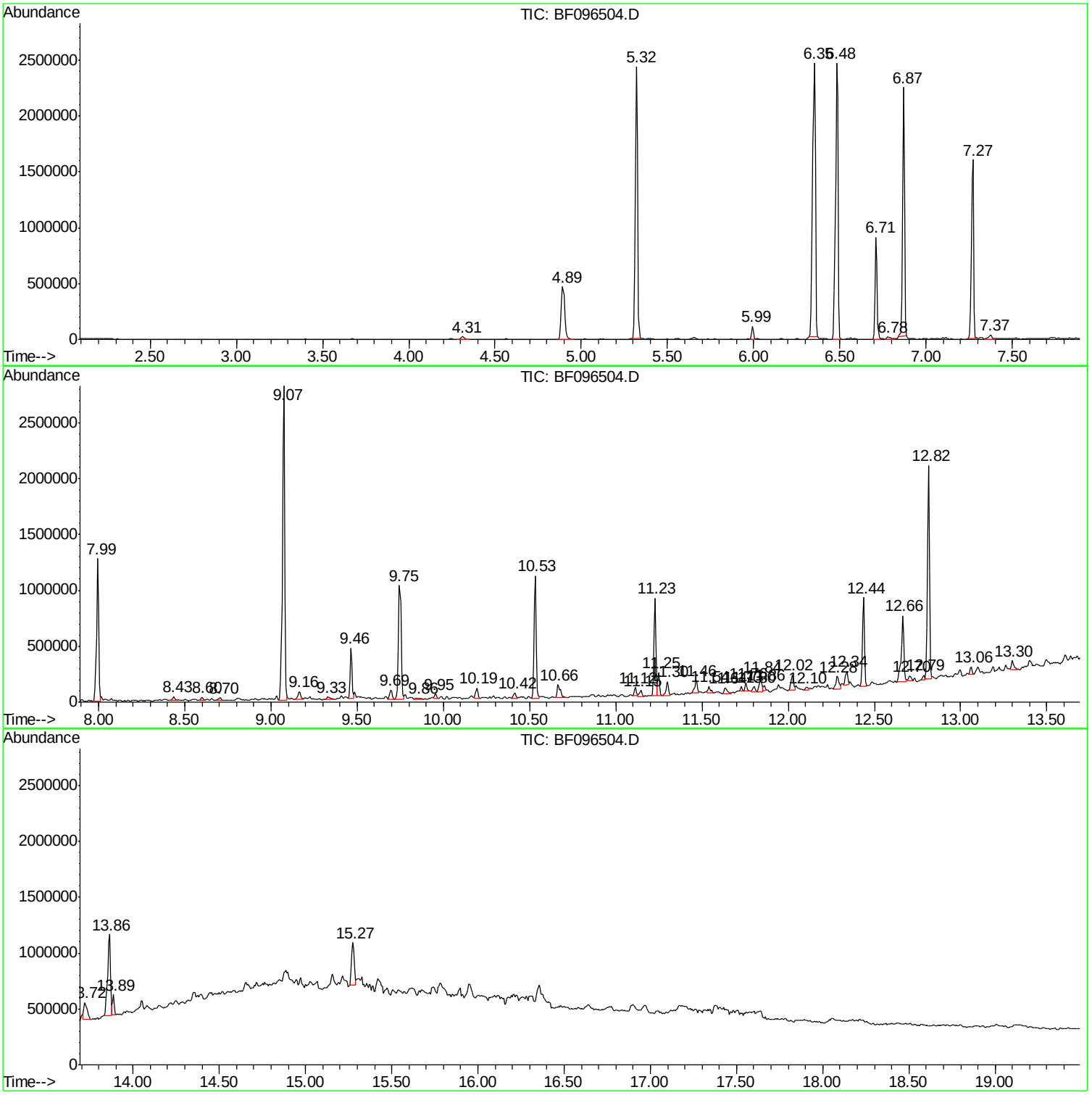
Sample : I3976-04
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B9-6-8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.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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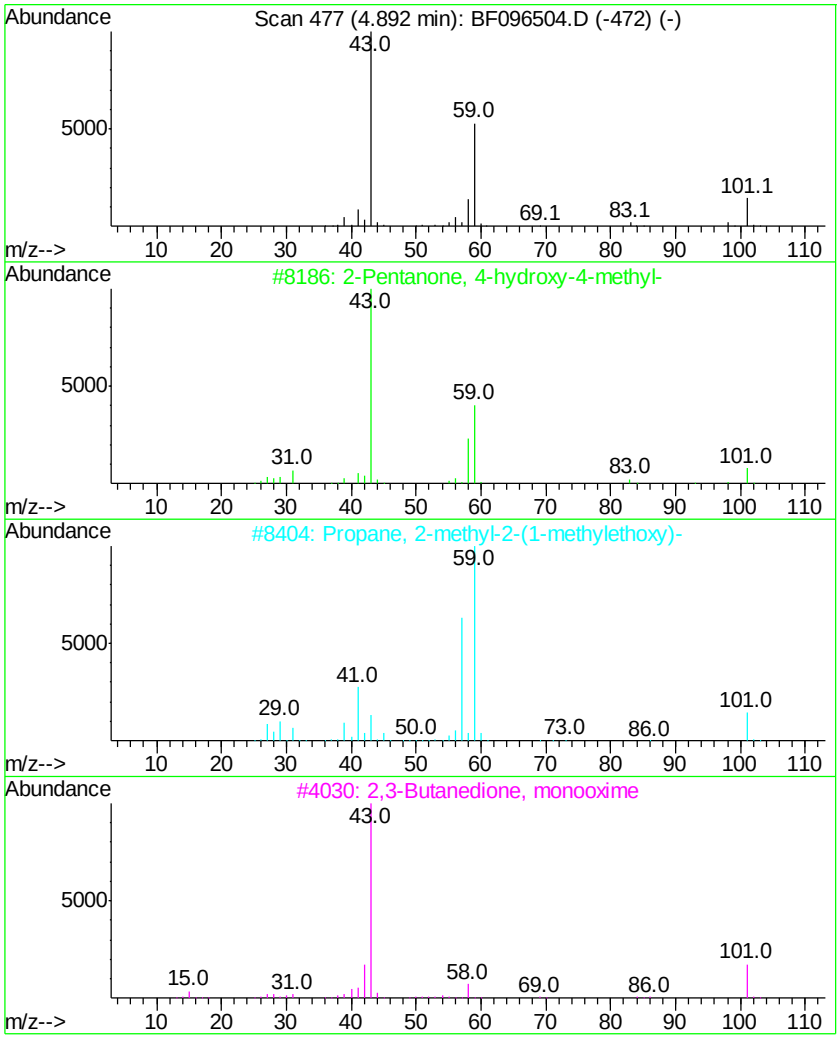
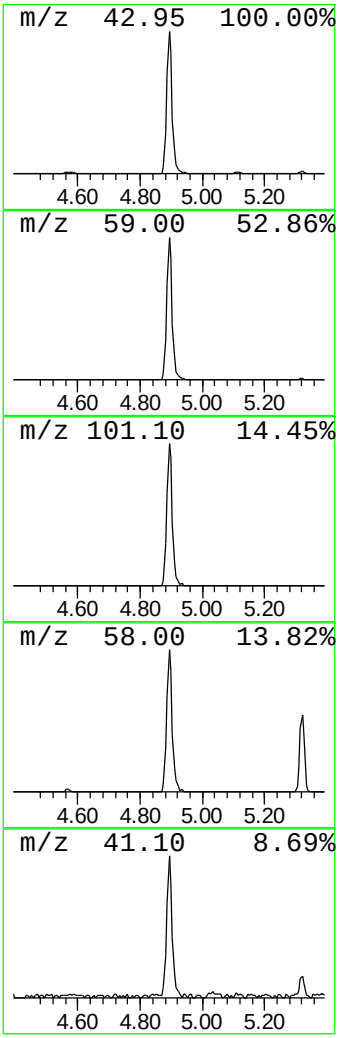
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.89	15.47 ng	588978	1,4-Dichlorobenzene-d4	6.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	38
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	Ethanol, pentamethyl-	116	C7H16O	000594-83-2	9
5	5-Oxohexanenitrile	111	C6H9NO	010412-98-3	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF070517\
Data File : BF096504.D
Acq On : 6 Jul 2017 1:29
Operator : SJ/MA
Sample : I3976-04
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B9-6-8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

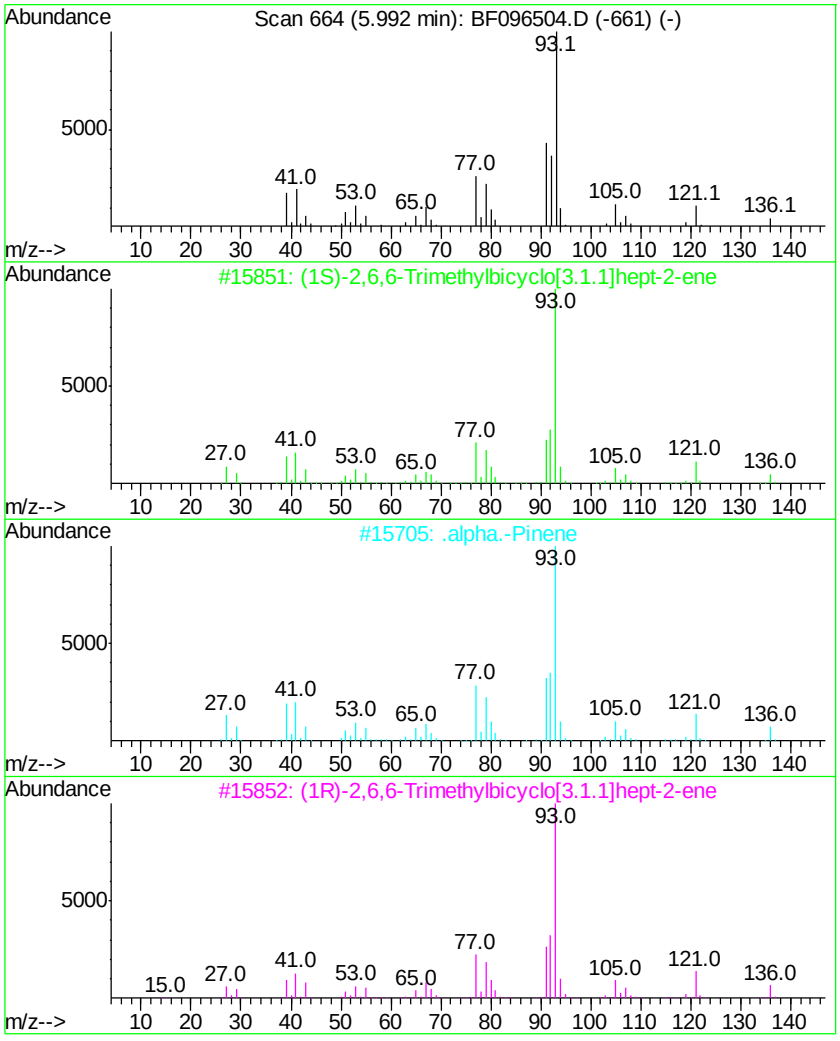
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

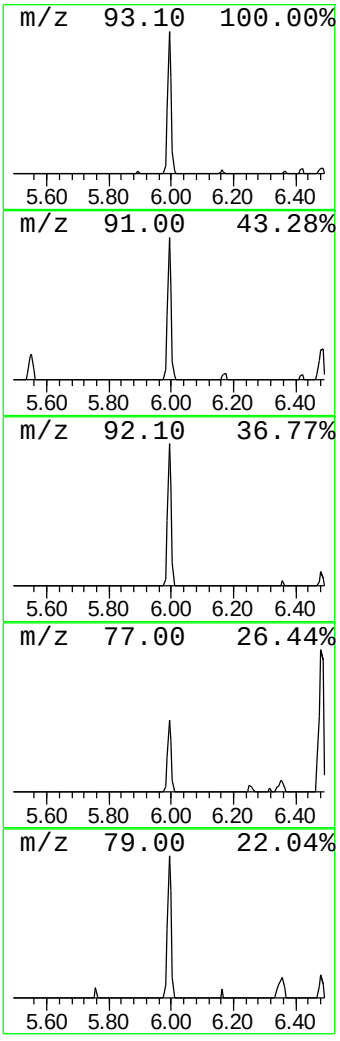
****

Peak Number 2 (1S)-2,6,6-Trimethylbicyclo... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.99	2.38 ng	90758	1,4-Dichlorobenzene-d4	6.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(1S)-2,6,6-Trimethylbicyclo[3.1....	136	C10H16	007785-26-4	96
2	.alpha.-Pinene	136	C10H16	000080-56-8	95
3	(1R)-2,6,6-Trimethylbicyclo[3.1....	136	C10H16	007785-70-8	94
4	Bicyclo[3.1.1]hept-2-ene, 3,6,6-...	136	C10H16	004889-83-2	91
5	1,3,6-Octatriene, 3,7-dimethyl-,...	136	C10H16	003338-55-4	91





Library Search Compound Report

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Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B9-6-8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
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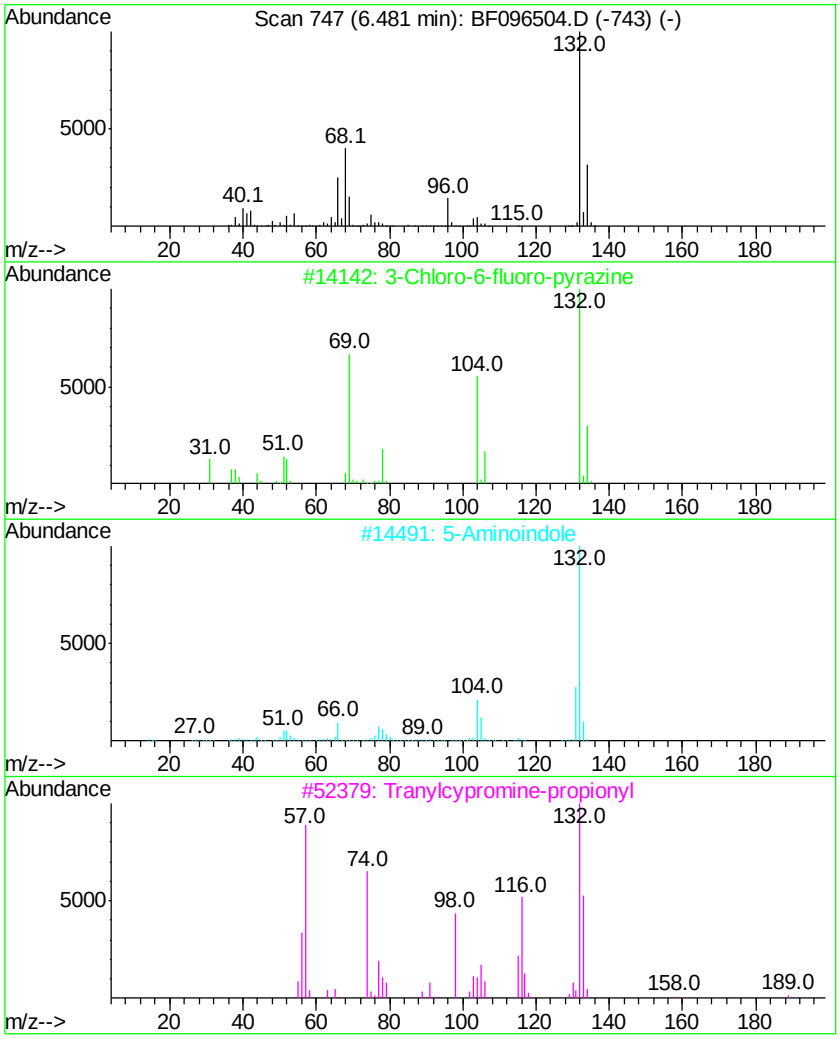
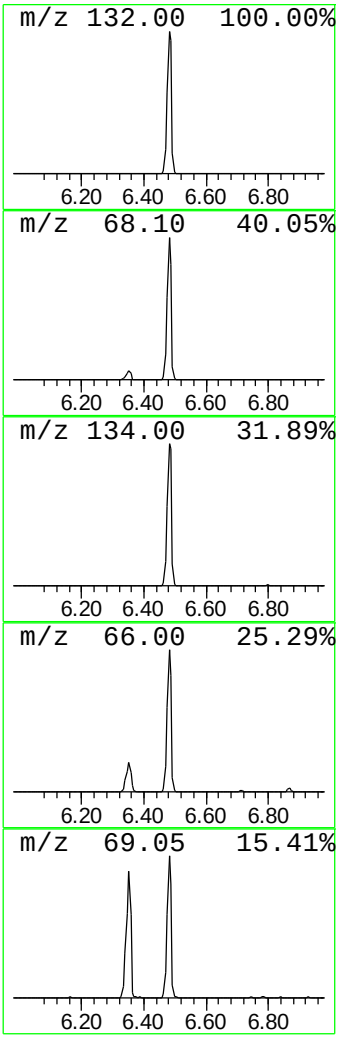
****

Peak Number 3 unknown6.48 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.48	63.83 ng	2430030	1,4-Dichlorobenzene-d4	6.71

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	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





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Instrument : BNA_F
ClientSampleId : B9-6-8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
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TIC Library : C:\DATABASE\NIST11.L
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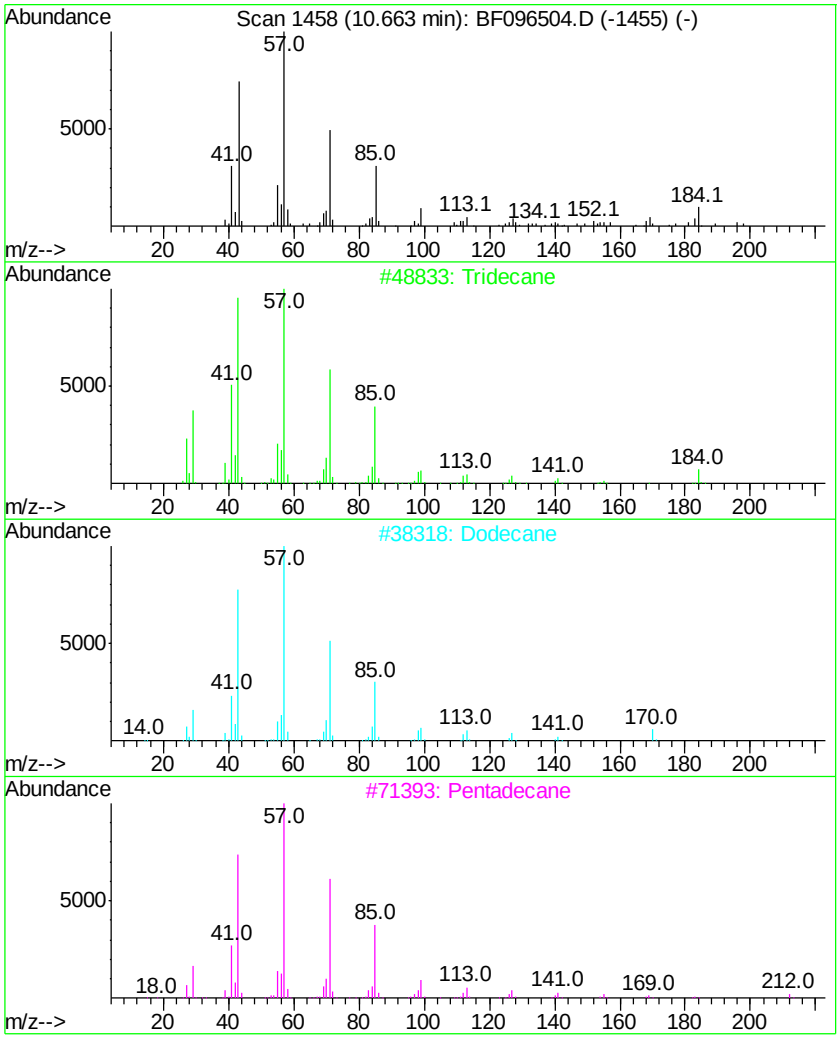
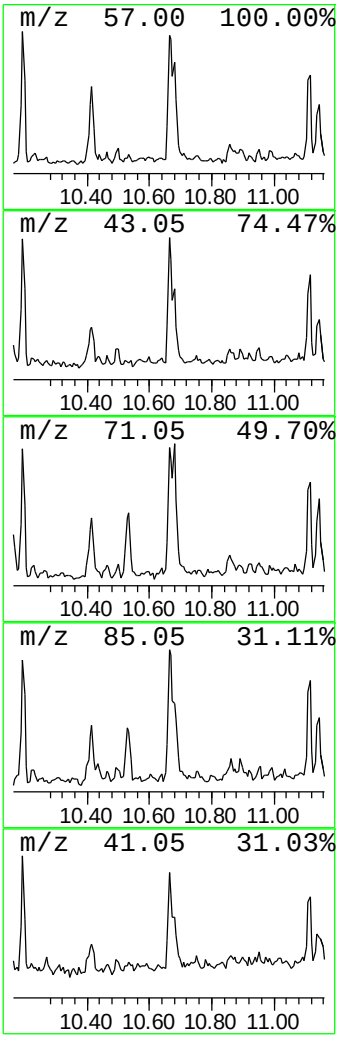
****

Peak Number 5 Tridecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.66	4.24 ng	159889	Phenanthrene-d10	11.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	72
2	Dodecane	170	C12H26	000112-40-3	68
3	Pentadecane	212	C15H32	000629-62-9	64
4	Hexadecane	226	C16H34	000544-76-3	64
5	Heptadecane	240	C17H36	000629-78-7	59





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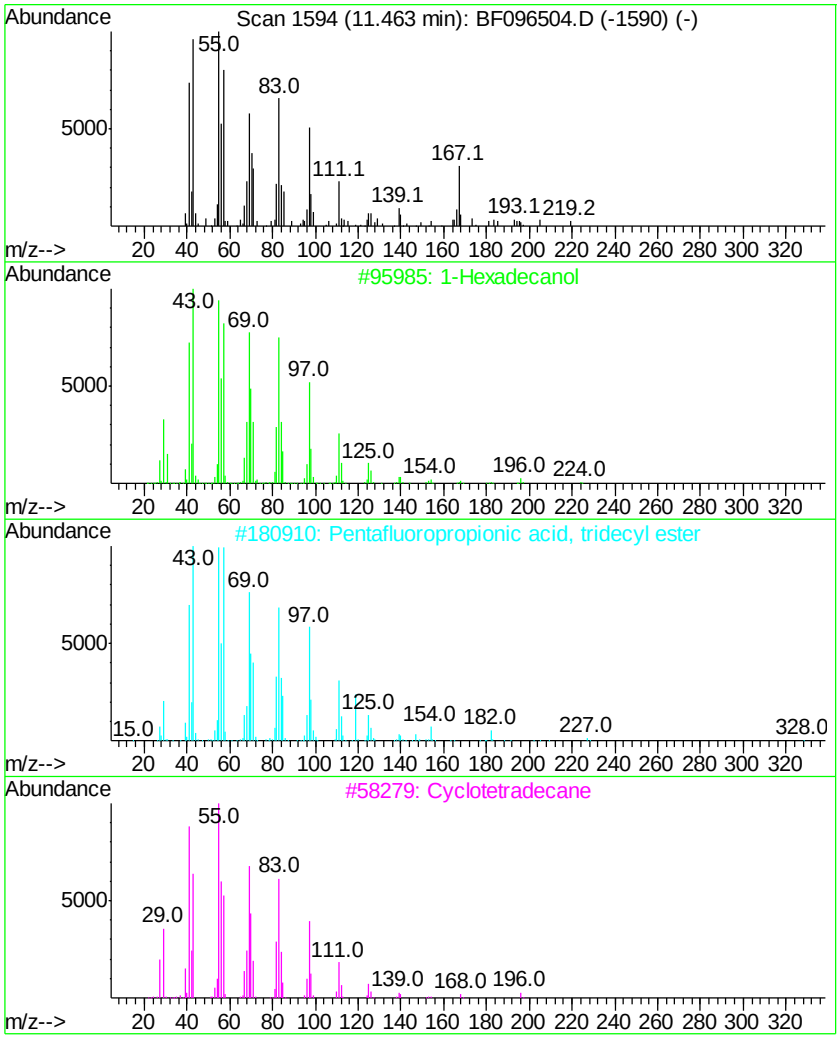
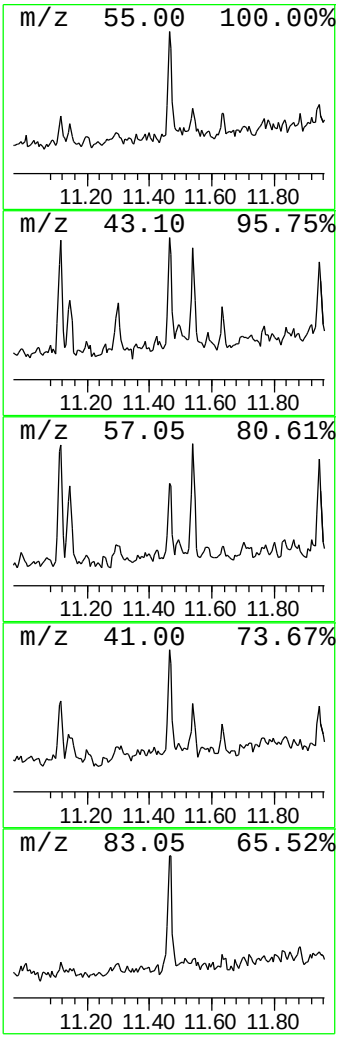
****

Peak Number 6 1-Hexadecanol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.46	3.29 ng	124083	Phenanthrene-d10	11.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexadecanol	242	C16H34O	036653-82-4	87
2	Pentafluoropropionic acid, tride...	346	C16H27F5O2	959261-22-4	87
3	Cyclotetradecane	196	C14H28	000295-17-0	86
4	Cyclododecane	168	C12H24	000294-62-2	86
5	2-Heptafluorobutyroxytetradecane	410	C18H29F7O2	1000245-49-7	76





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TIC Library : C:\DATABASE\NIST11.L
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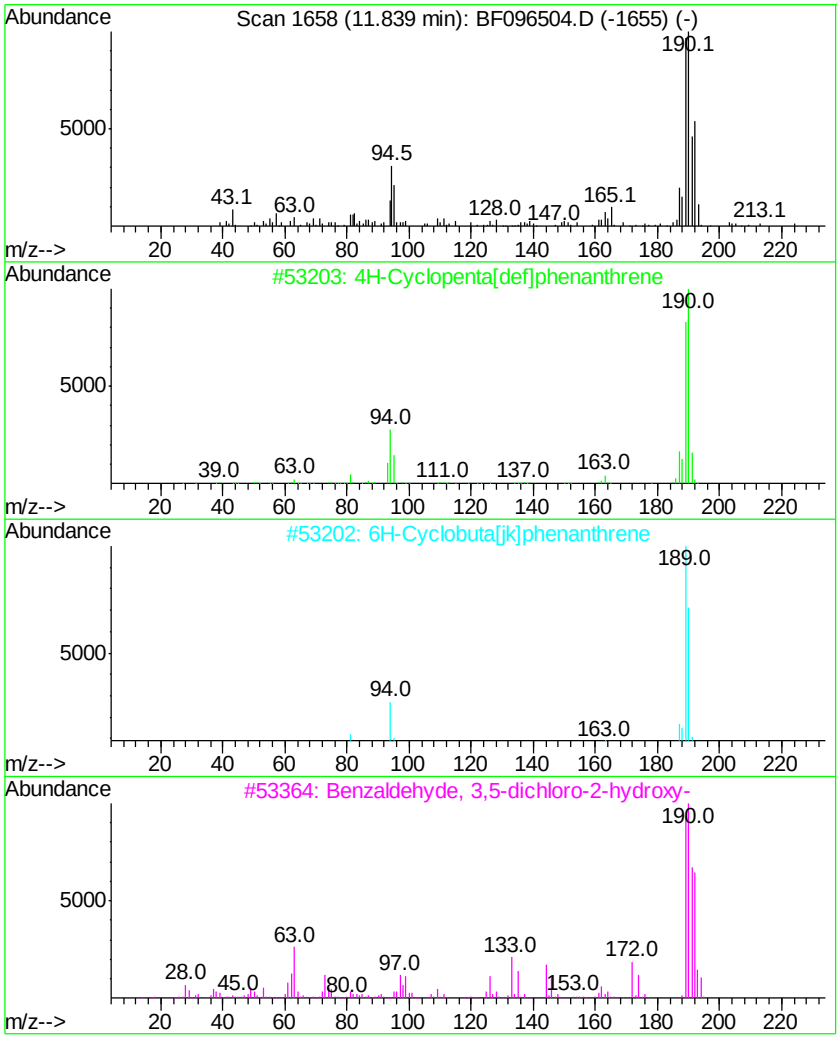
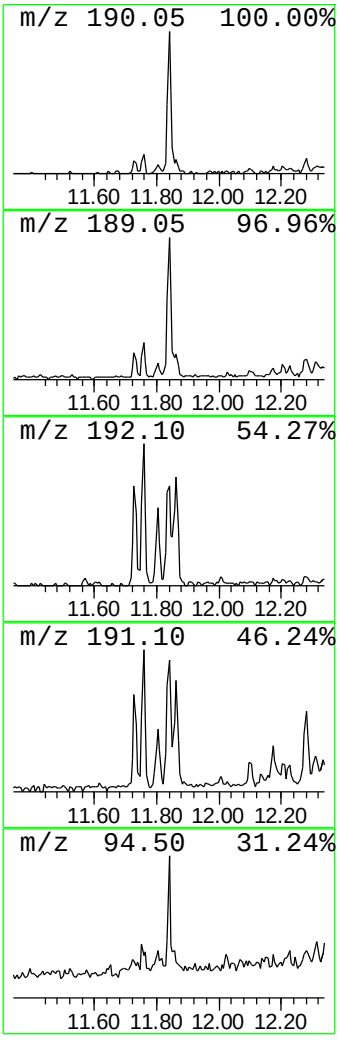
Peak Number 7 4H-Cyclopenta[def]phenanthrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.84	3.62 ng	136512	Phenanthrene-d10	11.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	76
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	50
3	Benzaldehyde, 3,5-dichloro-2-hyd...	190	C7H4Cl2O2	000090-60-8	47
4	Pyrazole-4-carboxaldehyde, 3-(4-...	190	C10H7FN2O	306936-57-2	43
5	Naphtho[1,2-b]norbornadiene	192	C15H12	1000210-14-8	22





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Misc :
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Instrument : BNA_F
ClientSampleId : B9-6-8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.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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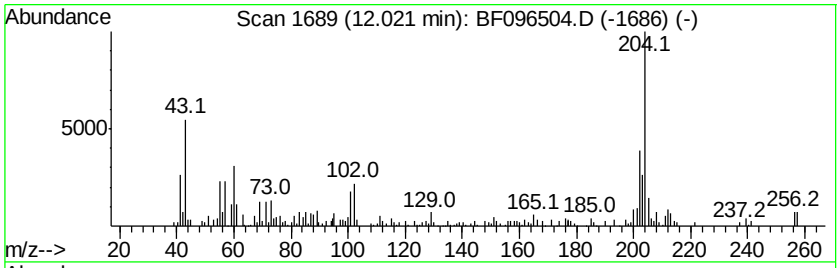
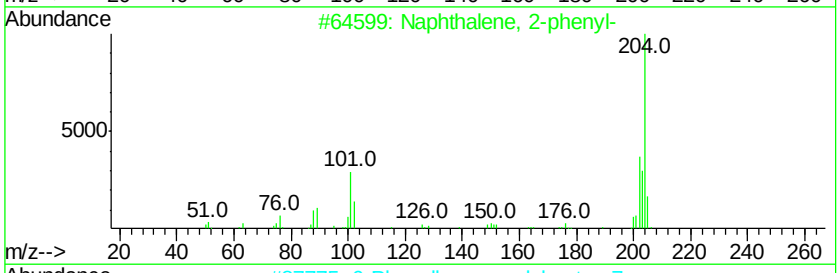
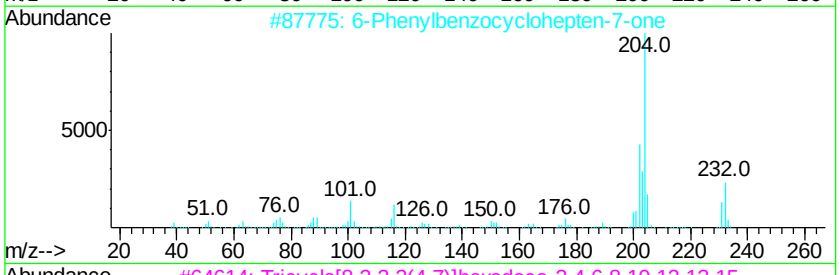
Peak Number 8 Naphthalene, 2-phenyl- Concentration Rank 8

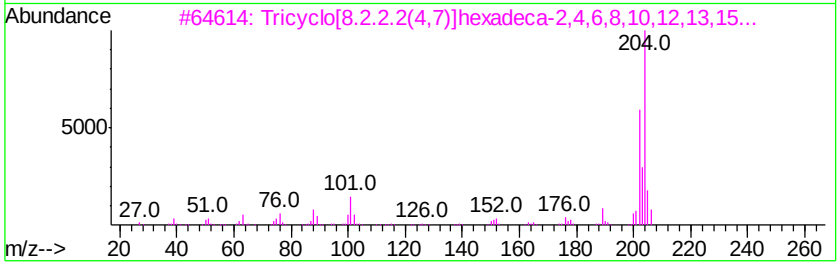
R.T.	EstConc	Area	Relative to ISTD	R.T.
12.02	3.59 ng	135273	Phenanthrene-d10	11.23

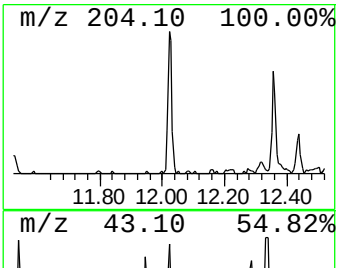
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2-phenyl-	204	C16H12	000612-94-2	60
2	6-Phenylbenzocyclohepten-7-one	232	C17H12O	093327-56-1	59
3	Tricyclo[8.2.2.2(4,7)]hexadeca-2...	204	C16H12	006572-60-7	55
4	5,16[1',2']:8,13[1'',2'']-Dibenz...	408	C32H24	005672-97-9	53
5	9,10-Bis(bromomethyl)anthracene	362	C16H12Br2	034373-96-1	49

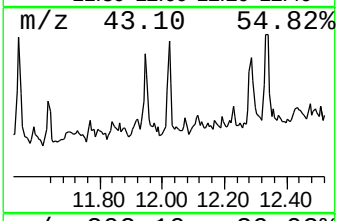


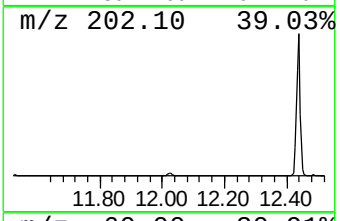


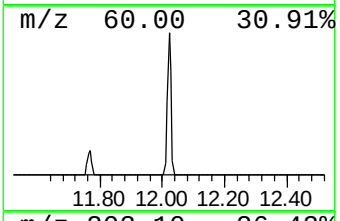


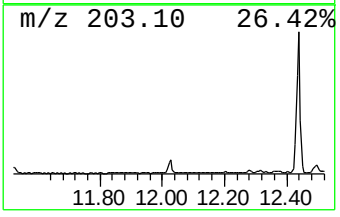












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Data File : BF096504.D
Acq On : 6 Jul 2017 1:29
Operator : SJ/MA
Sample : I3976-04
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B9-6-8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.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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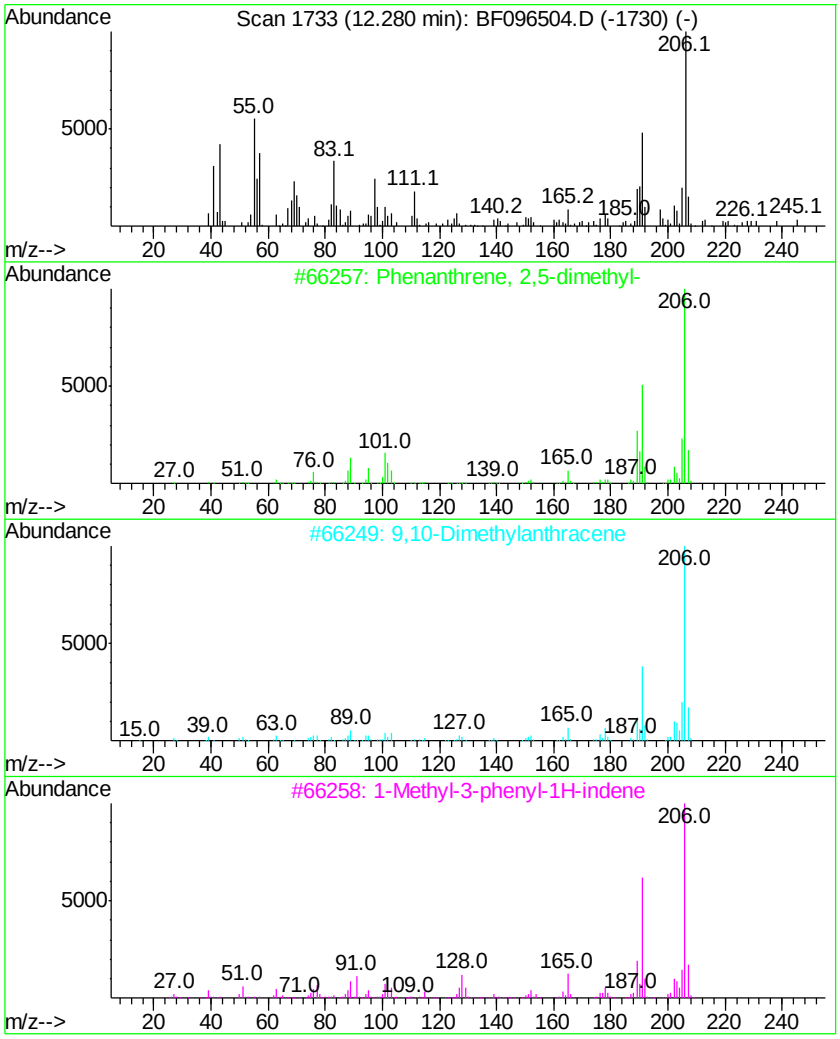
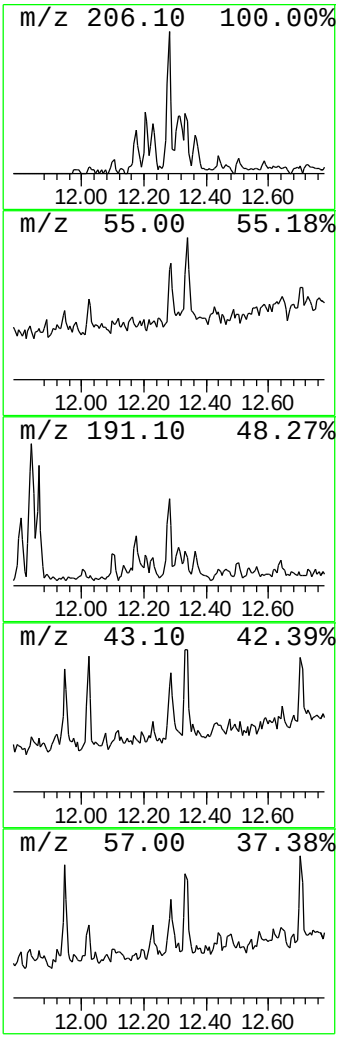
Peak Number 9 Phenanthrene, 2,5-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.28	3.78 ng	142368	Phenanthrene-d10	11.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	96
2	9,10-Dimethylanthracene	206	C16H14	000781-43-1	89
3	1-Methyl-3-phenyl-1H-indene	206	C16H14	022360-62-9	89
4	3-Methyl-1-phenyl-1H-indene	206	C16H14	022360-63-0	86
5	1,3-Diphenyl-3-methylcyclopropene	206	C16H14	086544-79-8	86





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Sample : I3976-04
Misc :
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ClientSampleId : B9-6-8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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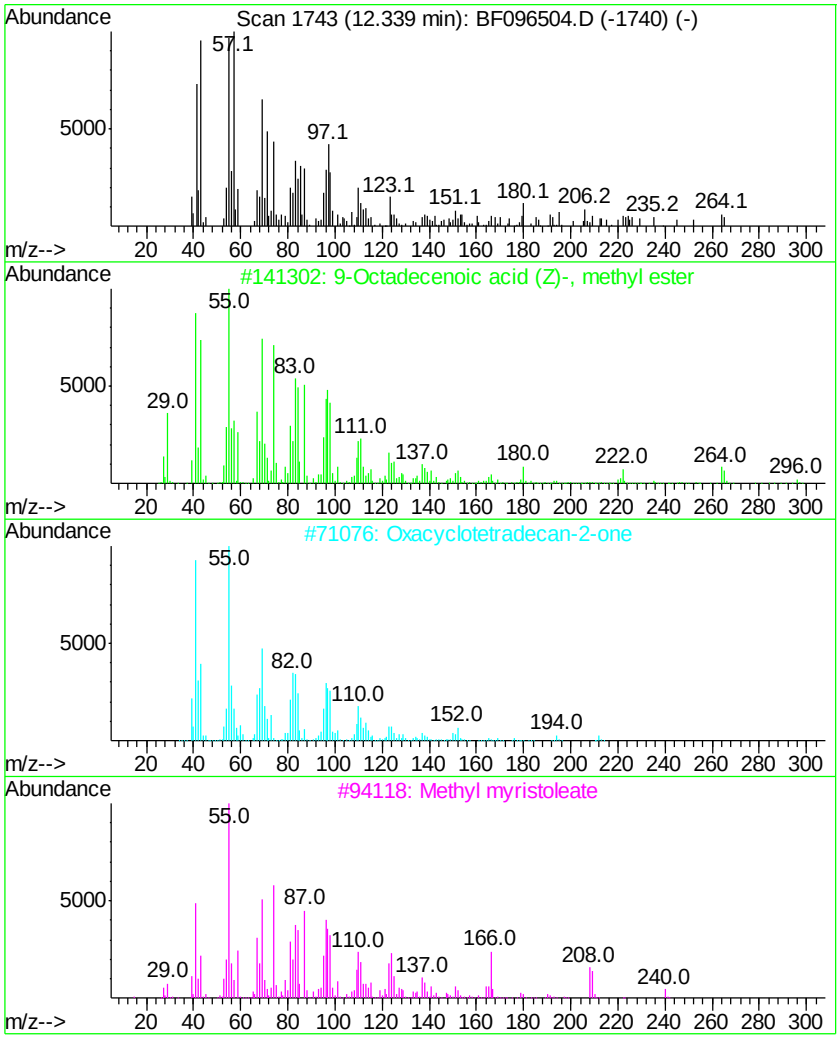
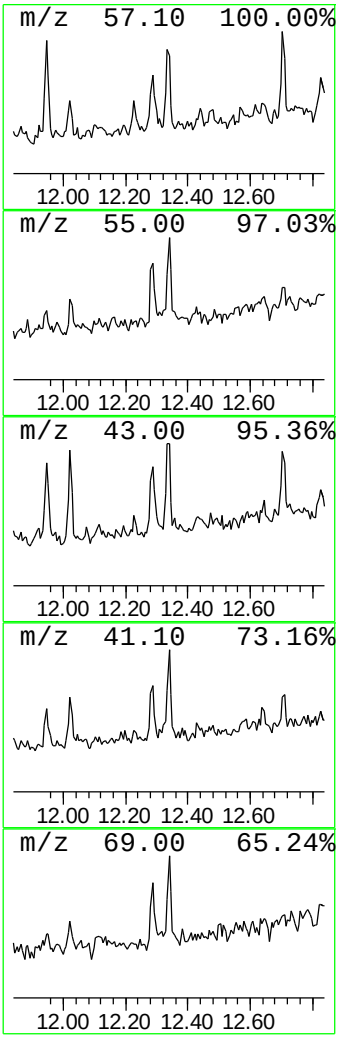
Peak Number 10 9-Octadecenoic acid (Z)-, m... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.34	2.80 ng	105448	Phenanthrene-d10	11.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	53
2	Oxacyclotetradecan-2-one	212	C13H24O2	001725-04-8	52
3	Methyl myristoleate	240	C15H28O2	056219-06-8	52
4	3-Decen-2-one	154	C10H18O	010519-33-2	41
5	Cetene	224	C16H32	000629-73-2	38





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Data File : BF096504.D
Acq On : 6 Jul 2017 1:29
Operator : SJ/MA
Sample : I3976-04
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B9-6-8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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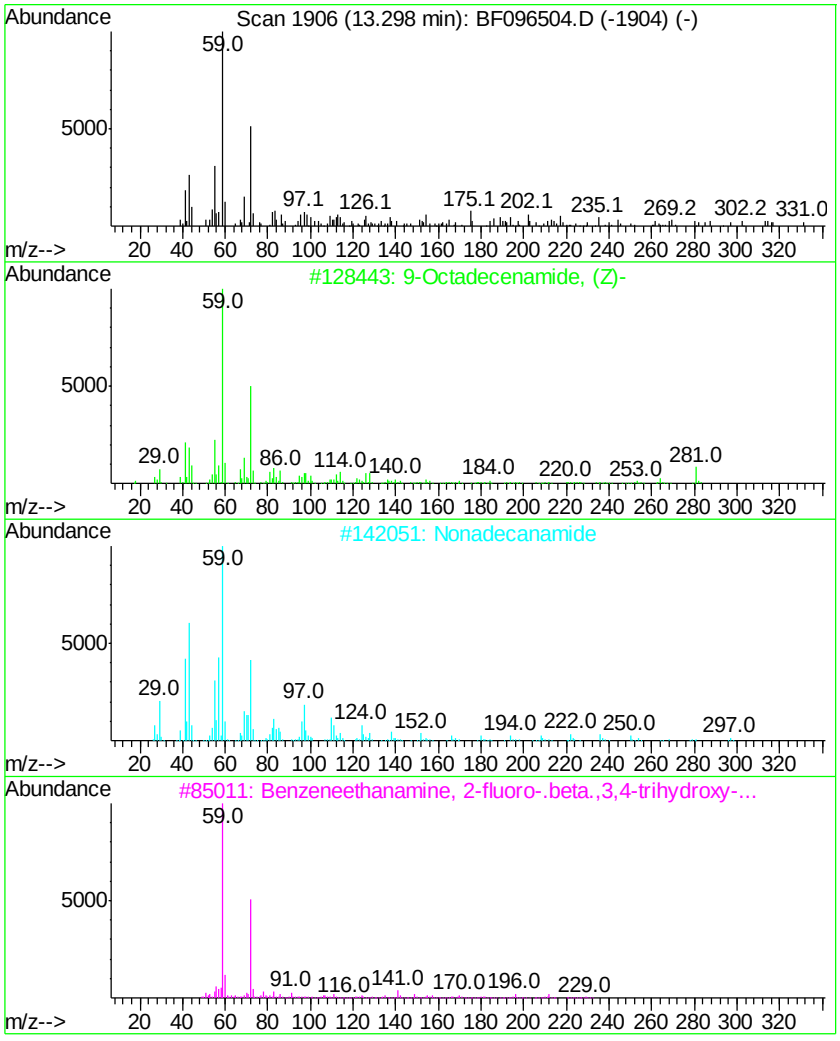
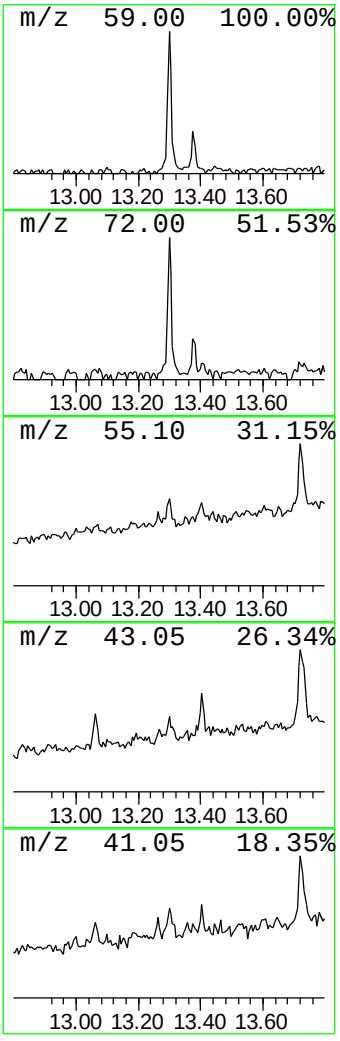
Peak Number 11 9-Octadecenamide, (Z)- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.30	2.04 ng	85922	Chrysene-d12	13.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	83
2	Nonadecanamide	297	C19H39NO	058185-32-3	80
3	Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FNO3	061338-98-5	64
4	Pentadecanamide, 15-bromo-	319	C15H30BrNO	1000163-86-1	53
5	7-Nonenamide	155	C9H17NO	090949-53-4	50





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Operator : SJ/MA
Sample : I3976-04
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B9-6-8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.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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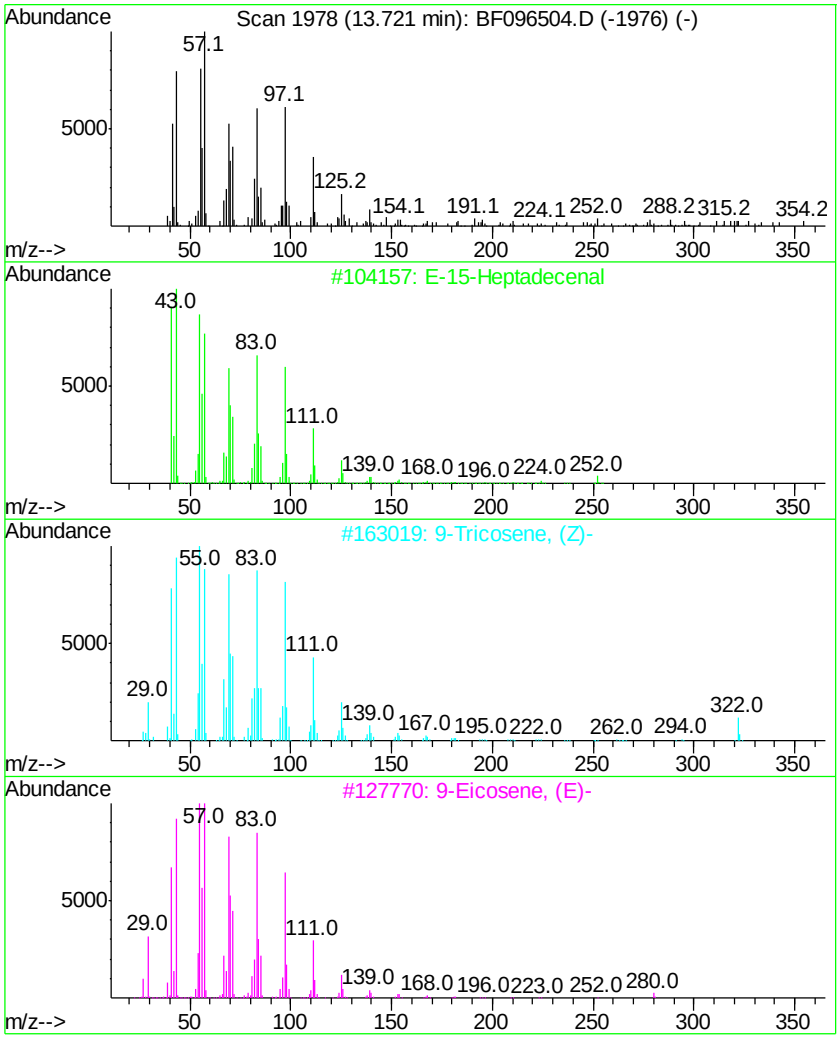
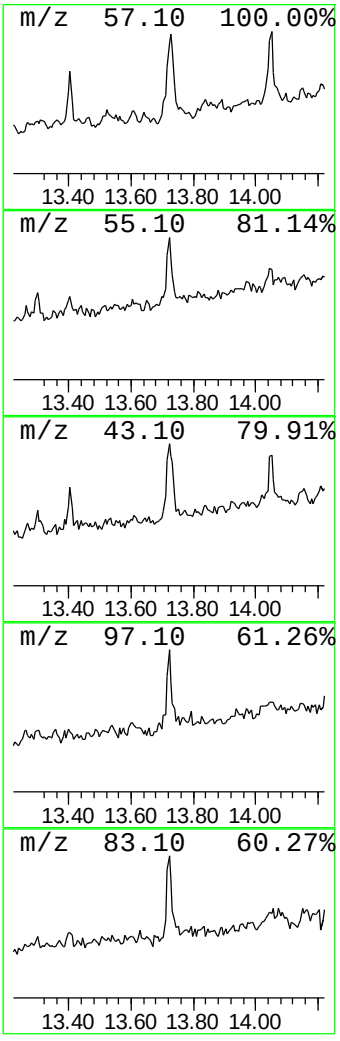
Peak Number 12 E-15-Heptadecenal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.72	4.27 ng	179819	Chrysene-d12	13.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	E-15-Heptadecenal	252	C17H32O	1000130-97-9	93
2	9-Tricosene, (Z)-	322	C23H46	027519-02-4	92
3	9-Eicosene, (E)-	280	C20H40	074685-29-3	91
4	5-Eicosene, (E)-	280	C20H40	074685-30-6	91
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070517\
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Acq On : 6 Jul 2017 1:29
Operator : SJ/MA
Sample : I3976-04
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B9-6-8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.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...	4.89	15.5	ng	588978	1	6.71	761386	20.0
(1S)-2,6,6-Trimet...	5.99	2.4	ng	90758	1	6.71	761386	20.0
unknown6.48	6.48	63.8	ng	2430030	1	6.71	761386	20.0
Tridecane	10.66	4.2	ng	159889	4	11.23	754187	20.0
1-Hexadecanol	11.46	3.3	ng	124083	4	11.23	754187	20.0
4H-Cyclopenta[def...	11.84	3.6	ng	136512	4	11.23	754187	20.0
Naphthalene, 2-ph...	12.02	3.6	ng	135273	4	11.23	754187	20.0
Phenanthrene, 2,5...	12.28	3.8	ng	142368	4	11.23	754187	20.0
9-Octadecenoic ac...	12.34	2.8	ng	105448	4	11.23	754187	20.0
9-Octadecenamide,...	13.30	2.0	ng	85922	5	13.86	842233	20.0
E-15-Heptadecenal	13.72	4.3	ng	179819	5	13.86	842233	20.0