LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF013117\
Data File : BF092696.D
Acq On : 31 Jan 2017 22:14
Operator : SJ/MA
Sample : I1596-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-19

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-BF013017.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	5.127	264	266	271	rBV	786001	885348	15.76%	2.030%
2	5.550	301	303	306	rBV	1847514	2452899	43.66%	5.624%
3	6.579	391	393	396	rBV	1464145	1528247	27.20%	3.504%
4	6.716	402	405	407	rBV	3713212	3529370	62.82%	8.092%
5	6.796	407	412	417	rVB5	31889	127778	2.27%	0.293%
6	6.944	422	425	427	rBV	1203429	1041839	18.54%	2.389%
7	7.105	436	439	441	rBV	3429029	3391350	60.36%	7.776%
8	7.516	471	475	477	rBV	2725978	3102100	55.21%	7.113%
9	7.562	477	479	481	rBV2	41054	60117	1.07%	0.138%
10	7.756	493	496	499	rVB	65246	94178	1.68%	0.216%
11	7.859	502	505	506	rBV	260993	357365	6.36%	0.819%
12	7.882	506	507	511	rVB	363492	343534	6.11%	0.788%
13	7.973	512	515	519	rVB	209580	218000	3.88%	0.500%
14	8.236	535	538	540	rBV	1490763	1341113	23.87%	3.075%
15	8.362	545	549	550	rBV3	37037	64468	1.15%	0.148%
16	8.476	556	559	561	rBV2	140723	247544	4.41%	0.568%
17	8.510	561	562	565	rVB	77584	77325	1.38%	0.177%
18	8.568	565	567	568	rBV	60829	60771	1.08%	0.139%
19	8.602	568	570	572	rVV2	40954	63241	1.13%	0.145%
20	8.659	572	575	579	rVB3	77430	137604	2.45%	0.316%
21	9.002	603	605	610	rVV4	32849	67787	1.21%	0.155%
22	9.082	610	612	615	rVB3	38955	66649	1.19%	0.153%
23	9.162	615	619	623	rBV5	46635	152190	2.71%	0.349%
24	9.242	623	626	627	rBV2	49154	72002	1.28%	0.165%
25	9.322	630	633	635	rBV	5107260	5618350	100.00%	12.882%
26	9.436	641	643	645	rVB3	51910	57493	1.02%	0.132%
27	9.505	648	649	651	rVB	75395	74869	1.33%	0.172%
28	9.539	651	652	655	rBV2	42516	66441	1.18%	0.152%
29	9.608	655	658	660	rVV2	59639	90220	1.61%	0.207%
30	9.653	660	662	664	rBV2	80281	107489	1.91%	0.246%
31	9.710	665	667	669	rVV	308416	281201	5.01%	0.645%
32	9.745	669	670	674	rVV4	40689	89779	1.60%	0.206%
33	9.813	674	676	677	rVV	55423	62651	1.12%	0.144%
34	9.848	677	679	682	rVV2	91837	149755	2.67%	0.343%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF013117\
Data File : BF092696.D
Acq On : 31 Jan 2017 22:14
Operator : SJ/MA
Sample : I1596-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-19

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-BF013017.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	9.996	690	692	695	rVB	1703163	1613771	28.72%	3.700%
36	10.065	695	698	700	rBV3	28992	63709	1.13%	0.146%
37	10.156	705	706	709	rBV	116627	168160	2.99%	0.386%
38	10.385	724	726	728	rBV2	58297	79870	1.42%	0.183%
39	10.671	749	751	754	rVB	192852	256371	4.56%	0.588%
40	10.796	759	762	764	rVV	2697838	2973369	52.92%	6.817%
41	10.853	764	767	770	rVV	131417	170890	3.04%	0.392%
42	10.911	770	772	775	rVV3	247607	390080	6.94%	0.894%
43	10.979	775	778	779	rVV	114940	196709	3.50%	0.451%
44	11.002	779	780	782	rVV2	144203	223400	3.98%	0.512%
45	11.036	782	783	785	rVV2	154836	201843	3.59%	0.463%
46	11.105	787	789	792	rVV2	92458	199401	3.55%	0.457%
47	11.151	792	793	795	rVB2	171897	185063	3.29%	0.424%
48	11.196	795	797	799	rBV	141734	253658	4.51%	0.582%
49	11.231	799	800	802	rVB	97582	94581	1.68%	0.217%
50	11.356	808	811	812	rBV2	111575	219370	3.90%	0.503%
51	11.379	812	813	815	rVB	251880	228801	4.07%	0.525%
52	11.494	820	823	825	rBV	1409095	1560351	27.77%	3.578%
53	11.665	836	838	840	rBV	198297	217464	3.87%	0.499%
54	11.699	840	841	845	rVB	70221	117843	2.10%	0.270%
55	11.894	854	858	862	rVB2	83320	172878	3.08%	0.396%
56	12.751	931	933	936	rBV	121606	169985	3.03%	0.390%
57	12.854	940	942	944	rVB	61858	63963	1.14%	0.147%
58	13.082	959	962	964	rBV	3497736	4805434	85.53%	11.018%
59	13.631	1008	1010	1012	rVB	321056	281864	5.02%	0.646%
60	13.962	1037	1039	1051	rBV2	91675	191329	3.41%	0.439%
61	14.122	1051	1053	1056	rVB	1262600	1189788	21.18%	2.728%
62	15.597	1179	1182	1186	rVB	713560	1044352	18.59%	2.395%
63	16.043	1219	1221	1226	rVB	55316	102521	1.82%	0.235%
64	16.557	1263	1266	1272	rVB2	43501	96573	1.72%	0.221%

Sum of corrected areas: 43614458

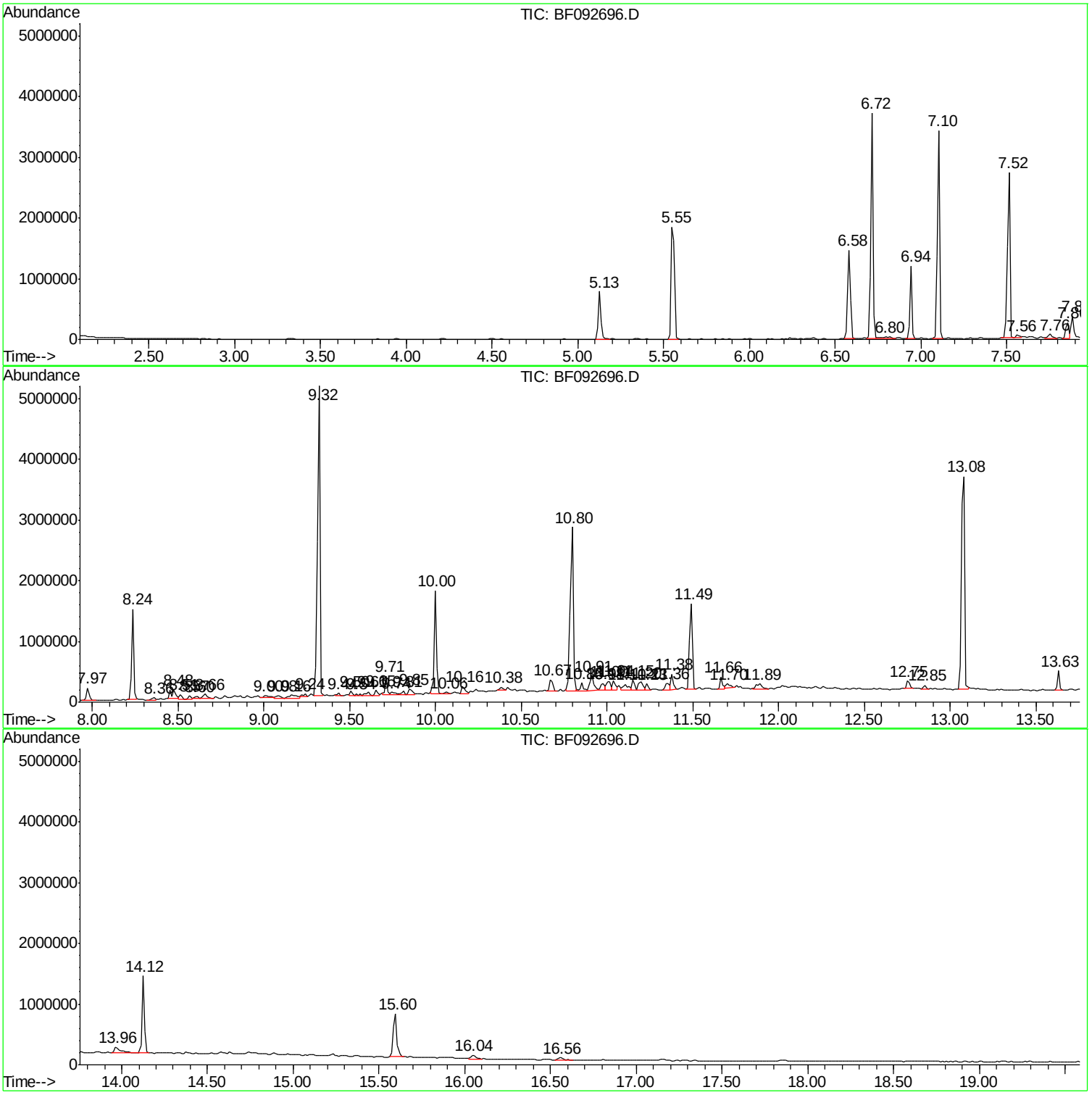
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF013117\
Data File : BF092696.D
Acq On : 31 Jan 2017 22:14
Operator : SJ/MA
Sample : I1596-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-19

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\HPCHEM1\BNA F\DATA\BF013117\
Data File : BF092696.D
Acq On : 31 Jan 2017 22:14
Operator : SJ/MA
Sample : I1596-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-19

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

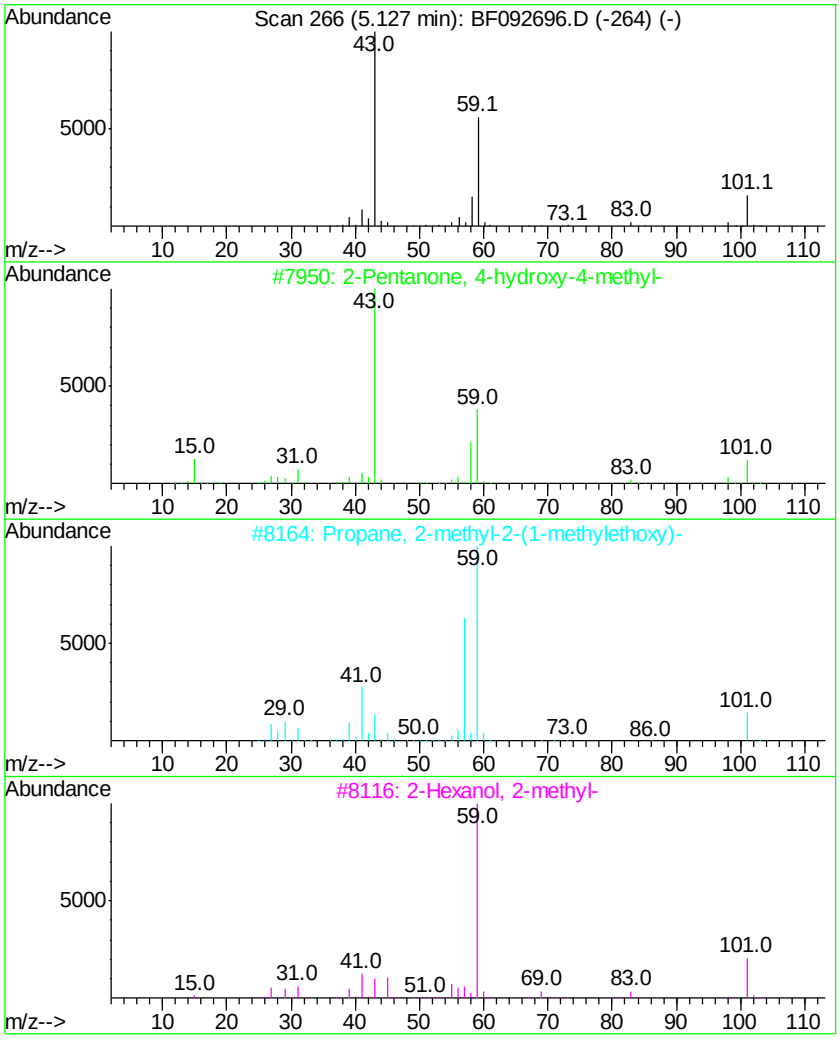
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

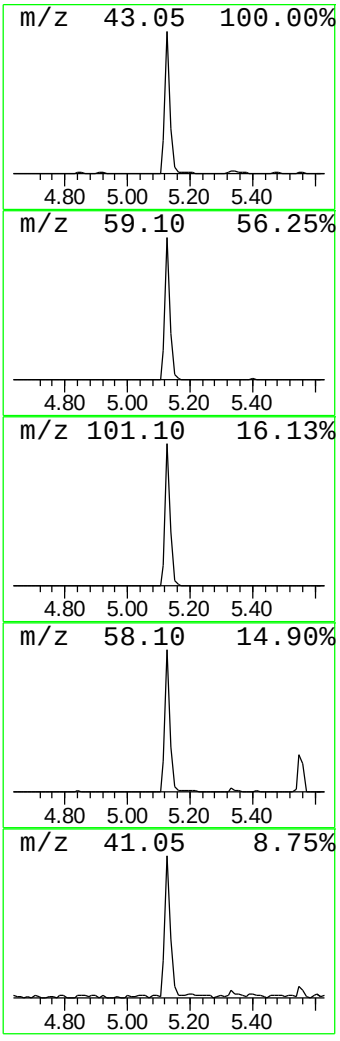
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.13	17.00 ng	885348	1,4-Dichlorobenzene-d4	6.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	40
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5	t-Butyl ethyl ether	102	C6H14O	1000118-18-4	23





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF013117\
Data File : BF092696.D
Acq On : 31 Jan 2017 22:14
Operator : SJ/MA
Sample : I1596-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-19

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

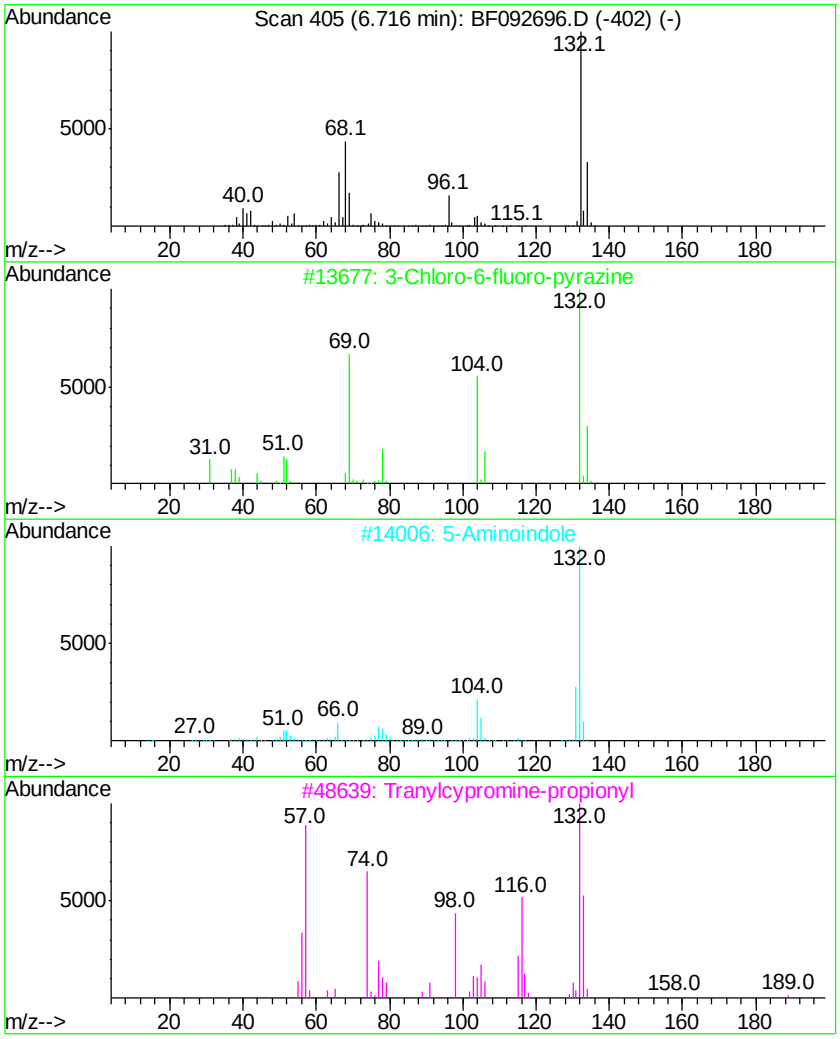
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

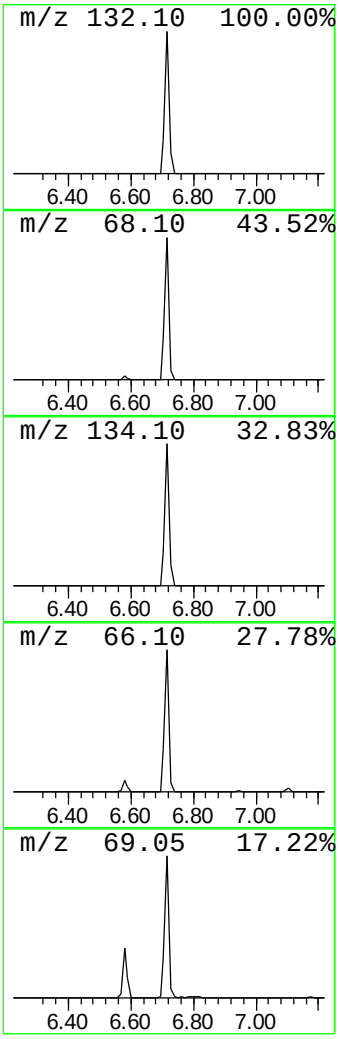
****

Peak Number 2 unknown6.72 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.72	67.75 ng	3529370	1,4-Dichlorobenzene-d4	6.94

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	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF013117\
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Acq On : 31 Jan 2017 22:14
Operator : SJ/MA
Sample : I1596-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-19

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

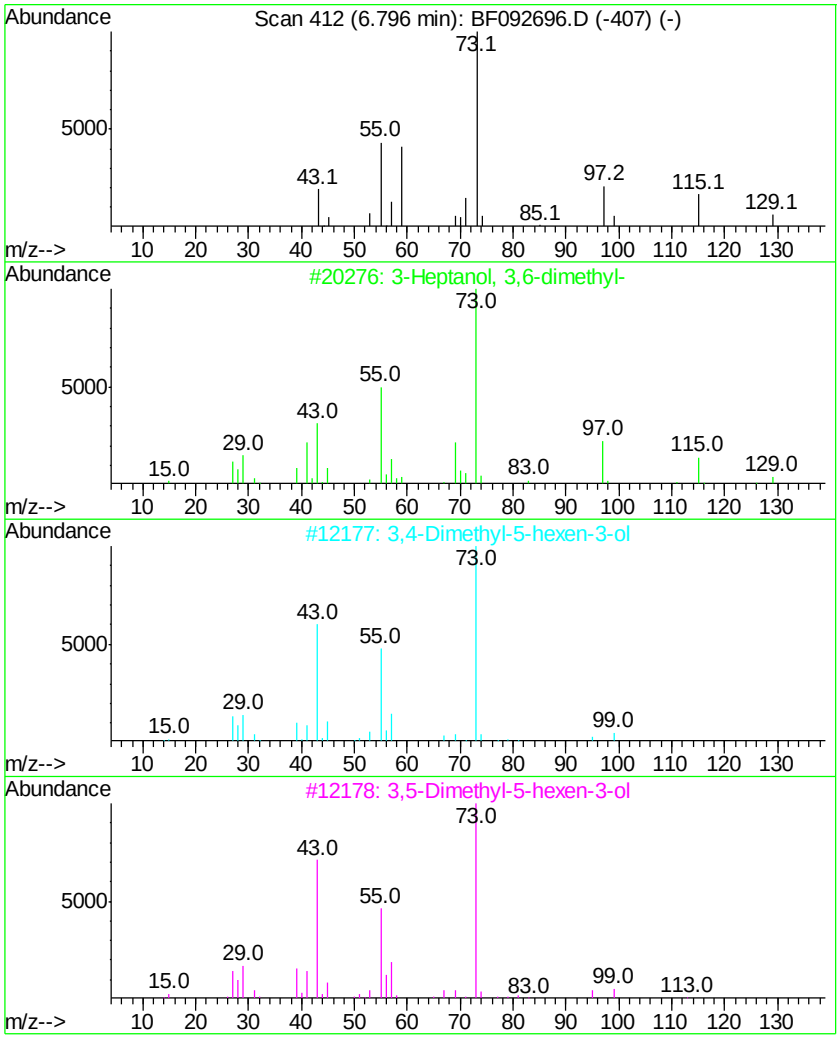
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

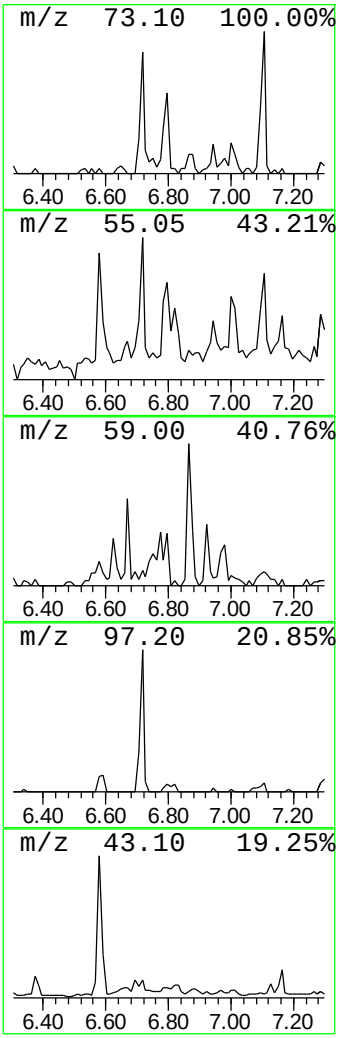
****

Peak Number 3 3-Heptanol, 3,6-dimethyl- Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.80	2.45 ng	127778	1,4-Dichlorobenzene-d4	6.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Heptanol, 3,6-dimethyl-	144	C9H20O	001573-28-0	50
2	3,4-Dimethyl-5-hexen-3-ol	128	C8H16O	001569-45-5	22
3	3,5-Dimethyl-5-hexen-3-ol	128	C8H16O	001569-46-6	10
4	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	9
5	3-Heptanol, 3,5-dimethyl-	144	C9H20O	019549-74-7	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF013117\
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Operator : SJ/MA
Sample : I1596-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-19

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

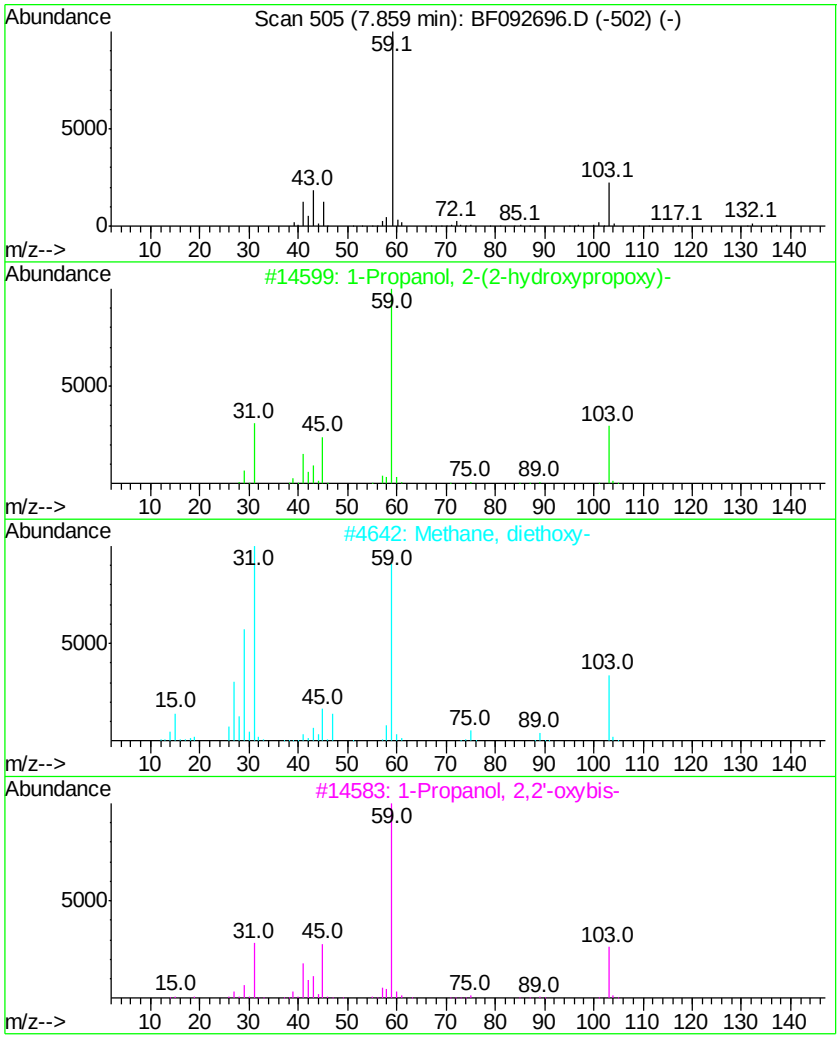
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

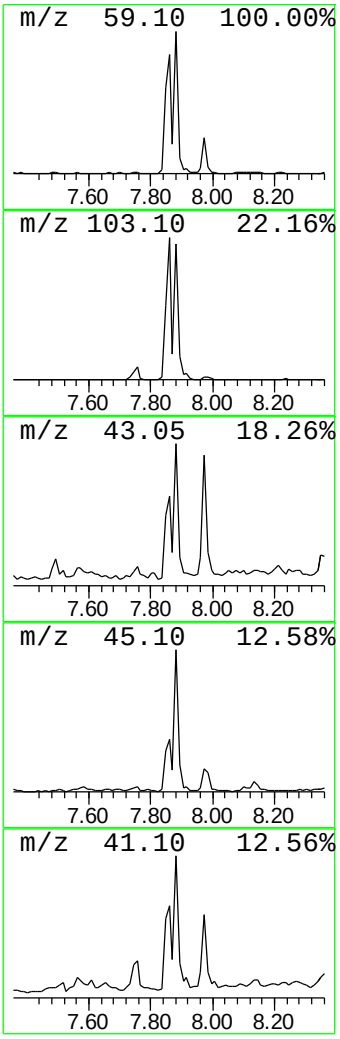
****

Peak Number 5 1-Propanol, 2-(2-hydroxypro... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.86	5.33 ng	357365	Naphthalene-d8	8.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	83
2	Methane, diethoxy-	104	C5H12O2	000462-95-3	78
3	1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	72
4	2-Propanol, 1,1'-[(1-methyl-1,2-...	192	C9H20O4	001638-16-0	64
5	2-Propanol, 1-[1-methyl-2-(2-pro...	174	C9H18O3	055956-25-7	64





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF013117\
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Sample : I1596-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-19

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

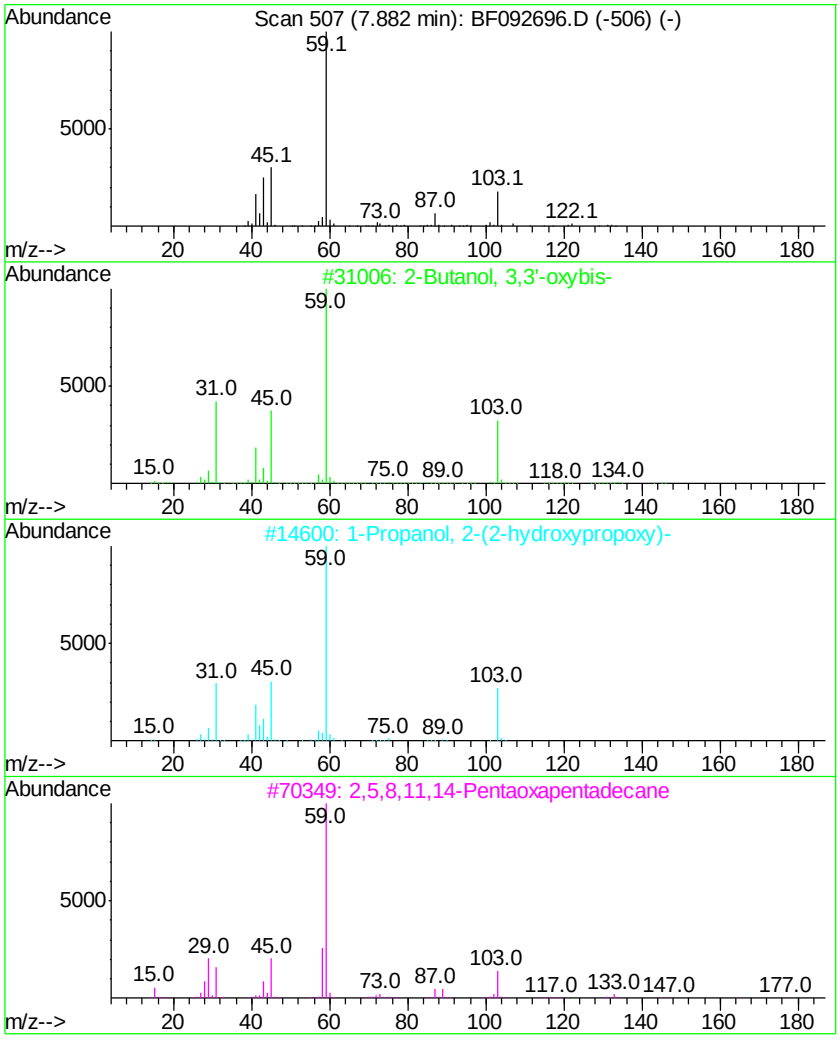
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

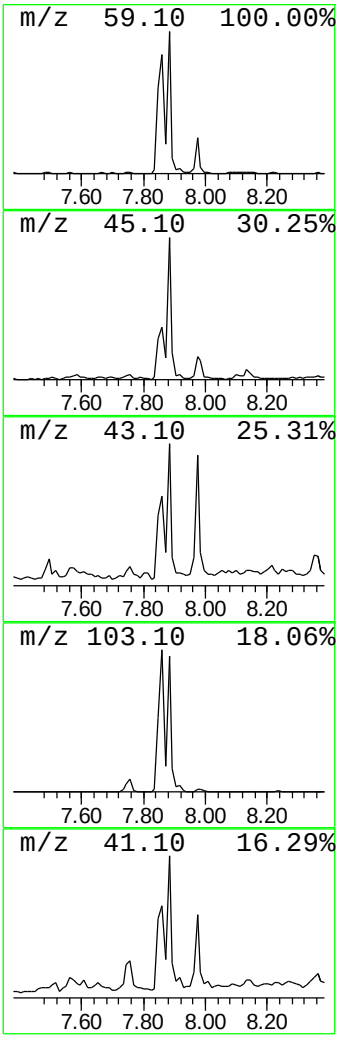
****

Peak Number 6 2-Butanol, 3,3'-oxybis- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.88	5.12 ng	343534	Naphthalene-d8	8.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanol, 3,3'-oxybis-	162	C8H18O3	054305-61-2	72
2	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	72
3	2,5,8,11,14-Pentaoxapentadecane	222	C10H22O5	000143-24-8	64
4	2-Pentanol, 2-methyl-	102	C6H14O	000590-36-3	64
5	1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	59





Data Path : Z:\HPCHEM1\BNA F\DATA\BF013117\
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Acq On : 31 Jan 2017 22:14
Operator : SJ/MA
Sample : I1596-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-19

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

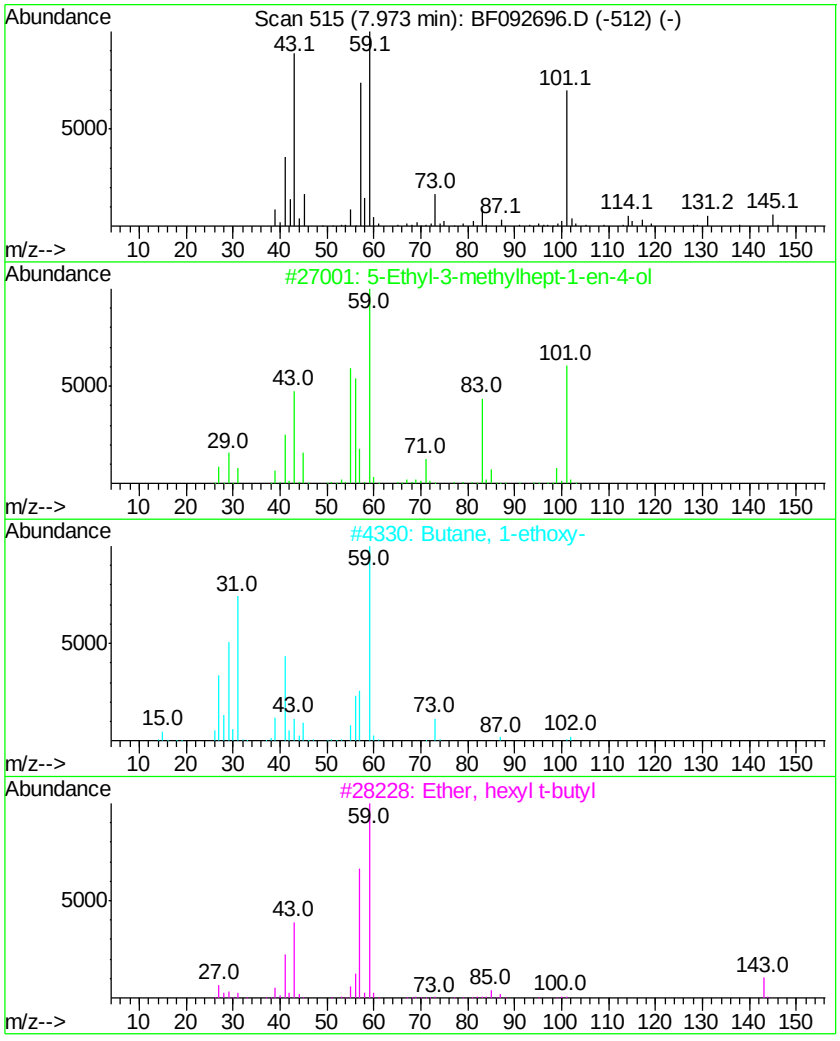
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

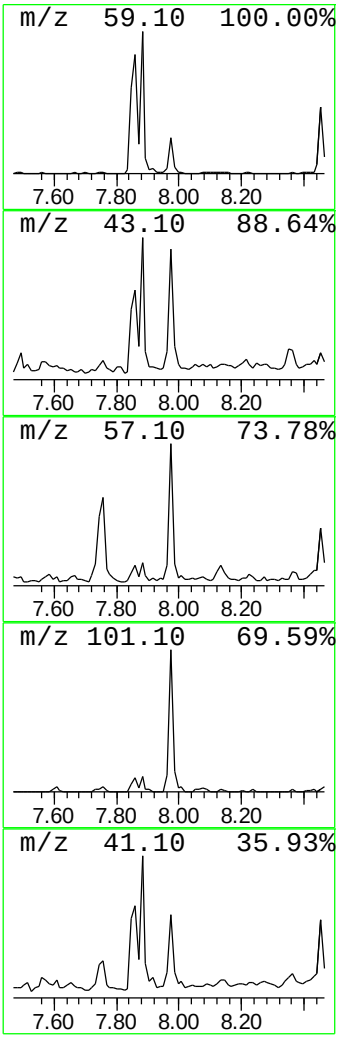
****

Peak Number 7 5-Ethyl-3-methylhept-1-en-4-ol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.97	3.25 ng	218000	Naphthalene-d8	8.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Ethyl-3-methylhept-1-en-4-ol	156	C10H20O	286424-80-4	53
2	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	43
3	Ether, hexyl t-butyl	158	C10H22O	069775-79-7	37
4	Butanedioic acid, monomethyl ester	132	C5H8O4	003878-55-5	27
5	Oxetane, 2,2,4-trimethyl-	100	C6H12O	023120-44-7	25





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF013117\
Data File : BF092696.D
Acq On : 31 Jan 2017 22:14
Operator : SJ/MA
Sample : I1596-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-19

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

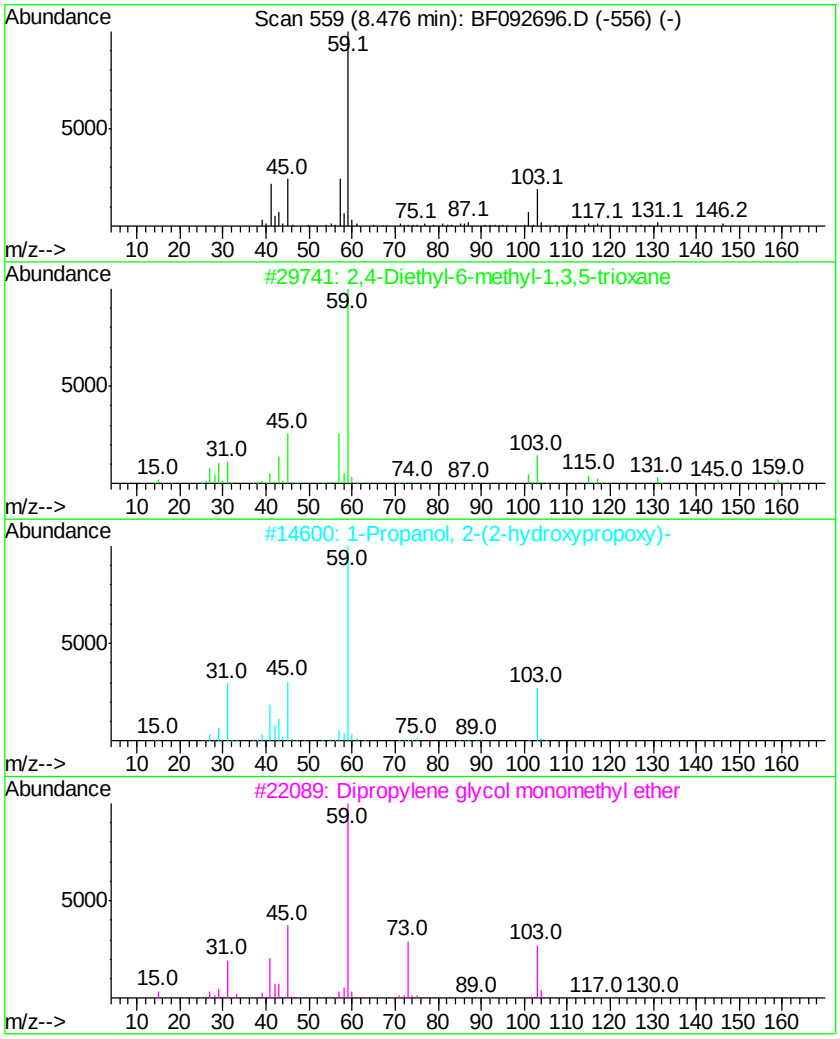
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

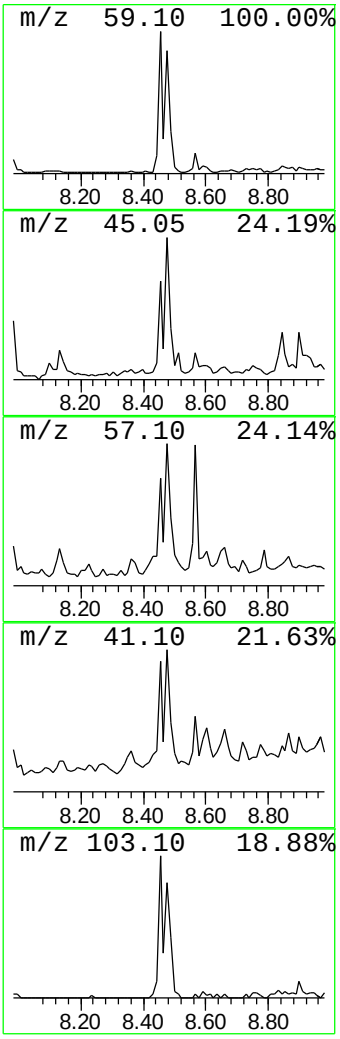
****

Peak Number 8 2,4-Diethyl-6-methyl-1,3,5-... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.48	3.69 ng	247544	Naphthalene-d8	8.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4-Diethyl-6-methyl-1,3,5-trioxane	160	C8H16O3	117888-04-7	78
2	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	72
3	Dipropylene glycol monomethyl ether	148	C7H16O3	034590-94-8	72
4	Pentane, 2-methoxy-	102	C6H14O	006795-88-6	64
5	2-Butanol, 3,3'-oxybis-	162	C8H18O3	054305-61-2	56





Data Path : Z:\HPCHEM1\BNA F\DATA\BF013117\
Data File : BF092696.D
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Sample : I1596-03
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ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-19

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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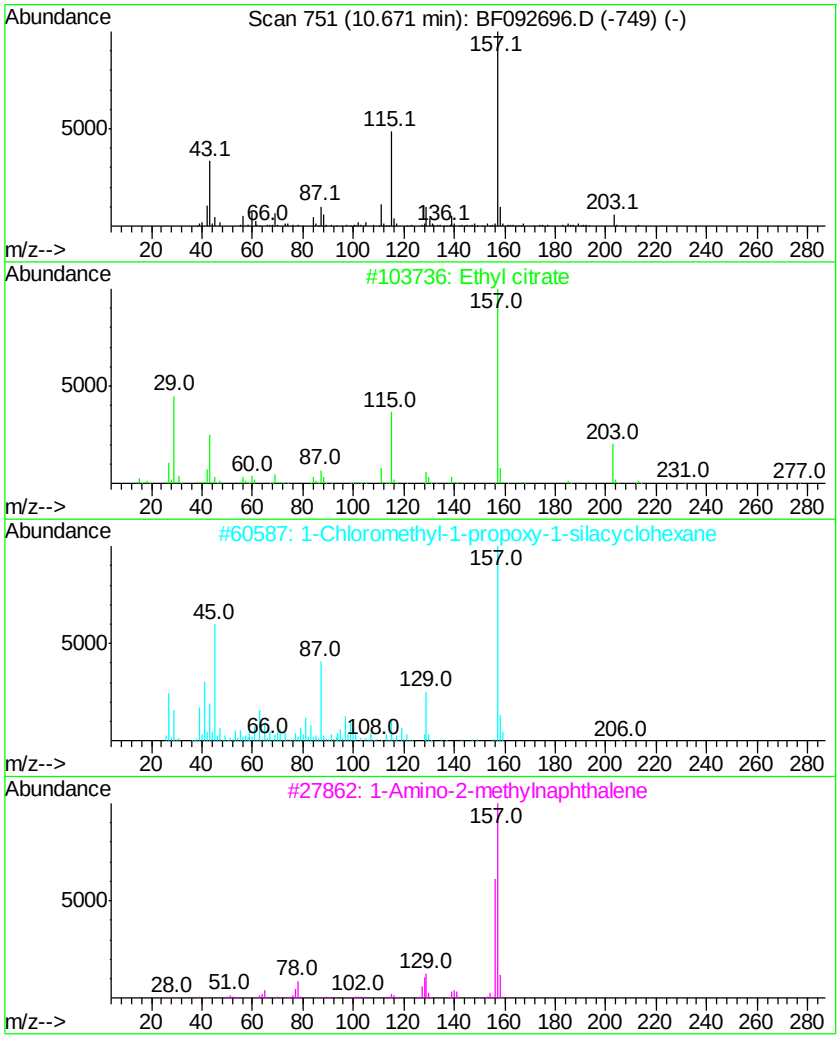
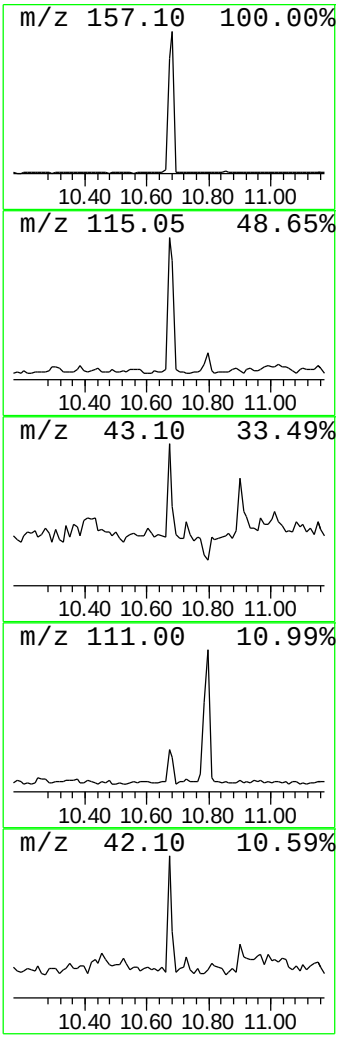
Peak Number 9 Ethyl citrate Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.67	3.18 ng	256371	Acenaphthene-d10	10.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethyl citrate	276	C12H20O7	000077-93-0	91
2	1-Chloromethyl-1-propoxy-1-silac...	206	C9H19ClOSi	1000279-33-1	43
3	1-Amino-2-methylnaphthalene	157	C11H11N	002246-44-8	43
4	Hexanedioic acid, 3-ethyl-, bis(...	286	C16H30O4	057983-54-7	40
5	1,3,2-Dioxaborinane, 4,6-dimethy...	200	C10H21BO3	052910-22-2	39





Library Search Compound Report

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Acq On : 31 Jan 2017 22:14
Operator : SJ/MA
Sample : I1596-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-19

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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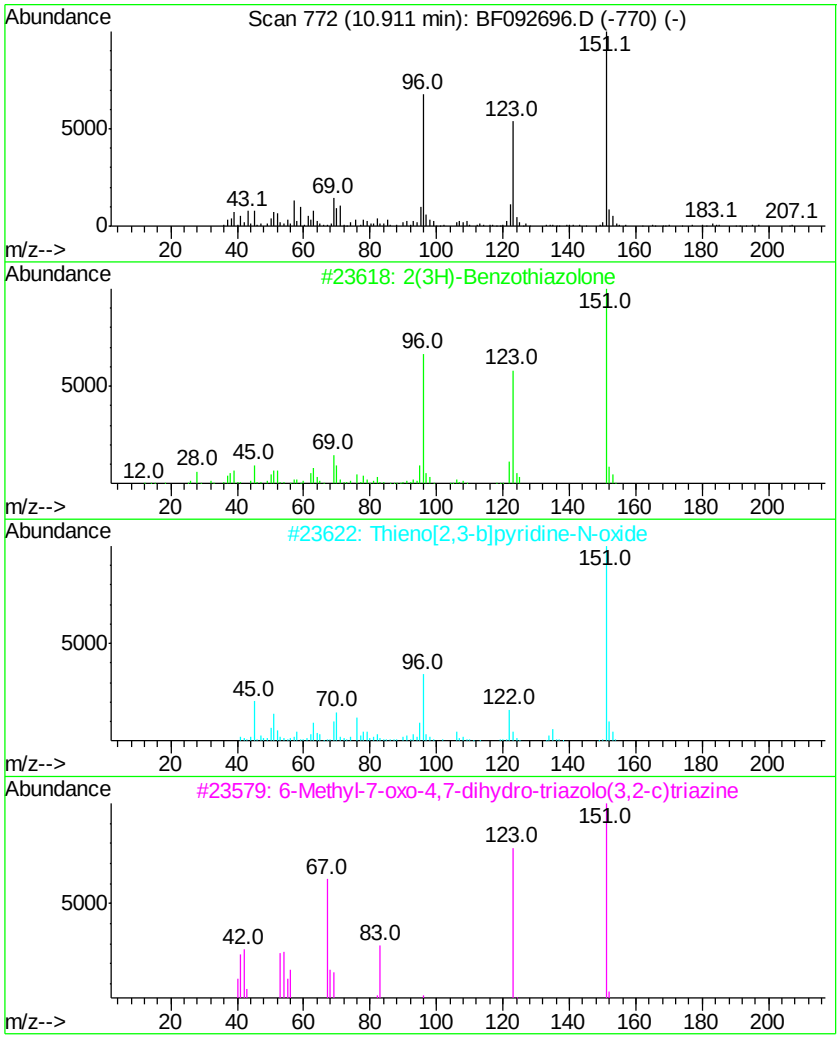
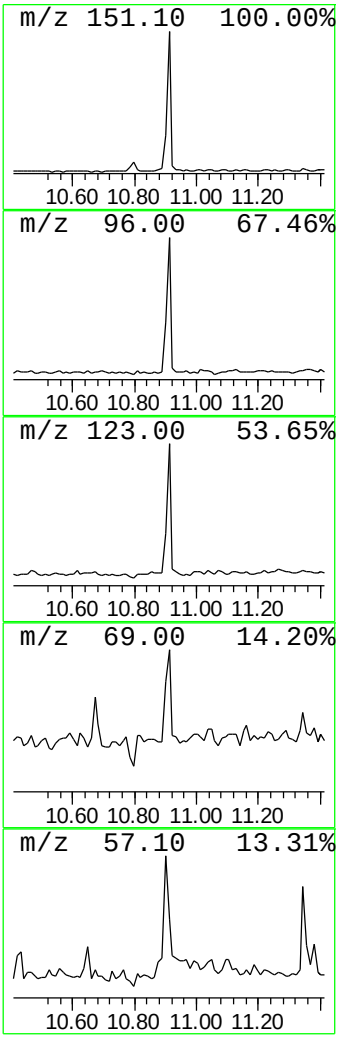
Peak Number 10 2(3H)-Benzothiazolone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.91	5.00 ng	390080	Phenanthrene-d10	11.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(3H)-Benzothiazolone	151	C7H5NOS	000934-34-9	93
2	Thieno[2,3-b]pyridine-N-oxide	151	C7H5NOS	025557-50-0	50
3	6-Methyl-7-oxo-4,7-dihydro-triaz...	151	C5H5N5O	057250-39-2	47
4	1,2-Benzisothiazol-3(2H)-one	151	C7H5NOS	002634-33-5	43
5	2(3H)-Benzoxazolethione	151	C7H5NOS	002382-96-9	38





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ClientSampleId : MW-19

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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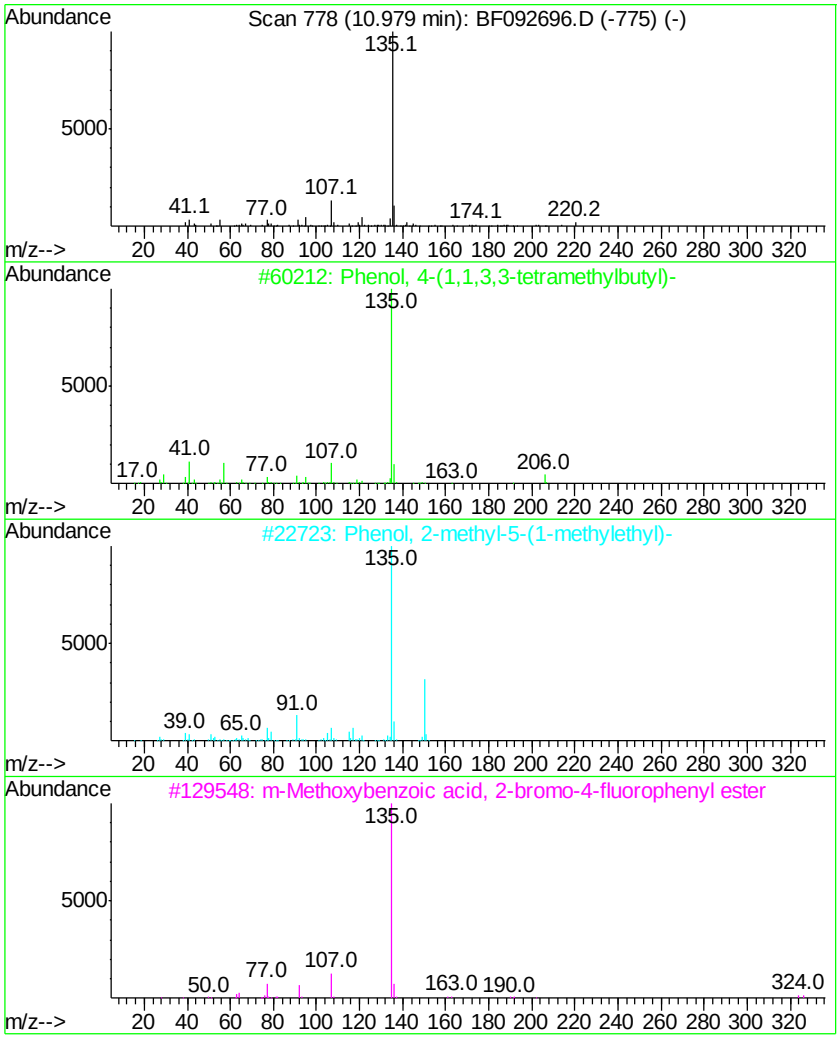
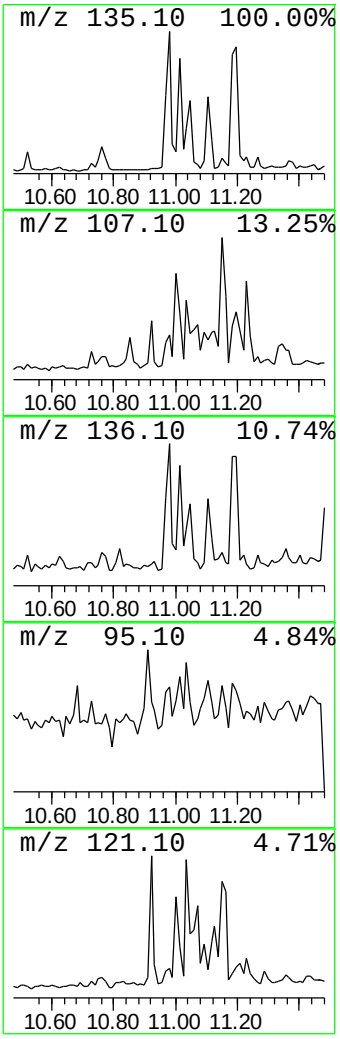
Peak Number 11 Phenol, 4-(1,1,3,3-tetramet... Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.98	2.52 ng	196709	Phenanthrene-d10	11.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-(1,1,3,3-tetramethylbu...	206	C14H22O	000140-66-9	78
2	Phenol, 2-methyl-5-(1-methylethyl)-	150	C10H14O	000499-75-2	72
3	m-Methoxybenzoic acid, 2-bromo-4...	324	C14H10BrFO3	1000292-63-0	64
4	1-n-Hexyladamantane	220	C16H28	022458-75-9	59
5	Pentanoic acid, 5-hydroxy-, p-t-...	250	C15H22O3	166273-37-6	56





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TIC Library : C:\DATABASE\NIST02.L
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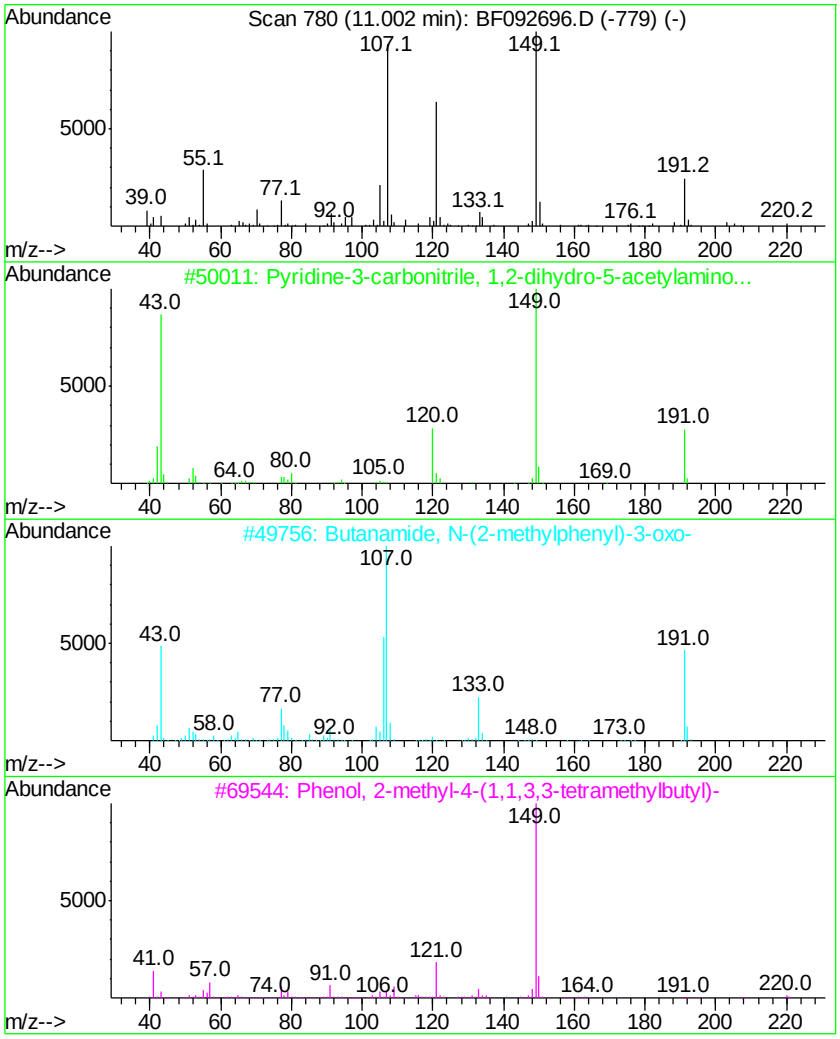
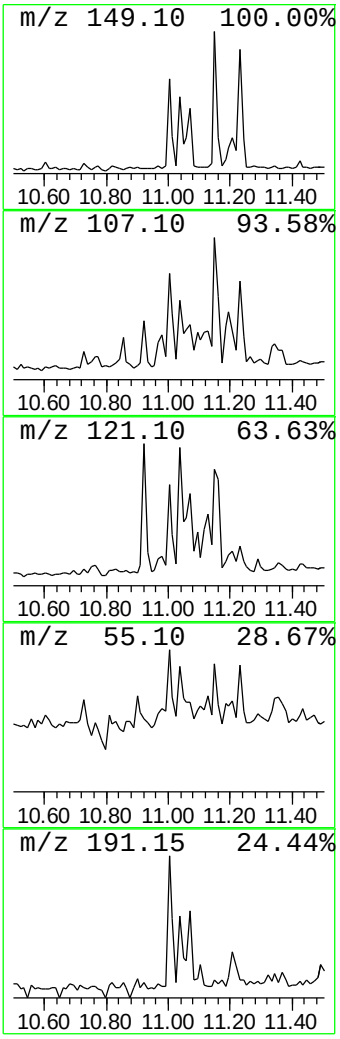
Peak Number 12 unknown11.00 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.00	2.86 ng	223400	Phenanthrene-d10	11.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyridine-3-carbonitrile, 1,2-dih...	191	C9H9N3O2	220098-92-0	43
2	Butanamide, N-(2-methylphenyl)-3...	191	C11H13NO2	000093-68-5	38
3	Phenol, 2-methyl-4-(1,1,3,3-tetr...	220	C15H24O	002219-84-3	38
4	2-Acetylbenzoic acid	164	C9H8O3	000577-56-0	38
5	1-(2,6-Dimethyl-4-propoxyphenyl)...	220	C14H20O2	1000190-22-3	38





Library Search Compound Report

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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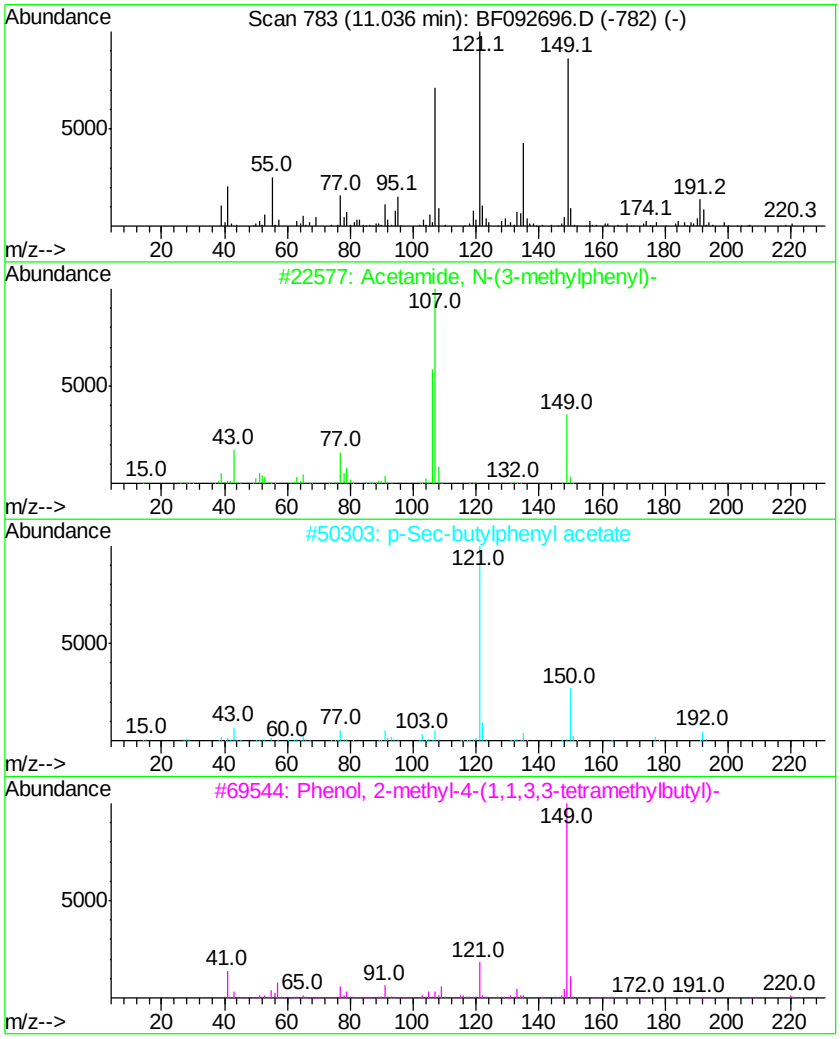
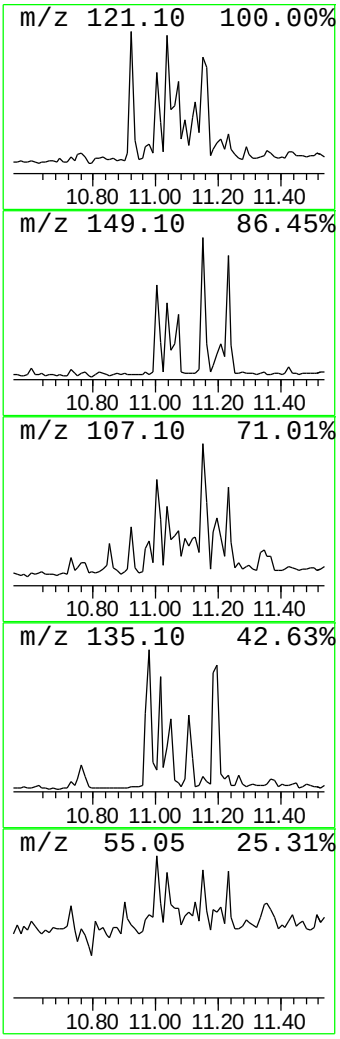
Peak Number 13 unknown11.04 Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.04	2.59 ng	201843	Phenanthrene-d10	11.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetamide, N-(3-methylphenyl)-	149	C9H11NO	000537-92-8	38
2	p-Sec-butylphenyl acetate	192	C12H16O2	003245-24-7	25
3	Phenol, 2-methyl-4-(1,1,3,3-tetr...	220	C15H24O	002219-84-3	25
4	3',4'-Formoxylidide	149	C9H11NO	006639-60-7	25
5	Phenol, 2-ethyl-4-methyl-	136	C9H12O	003855-26-3	22





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Instrument : BNA_F
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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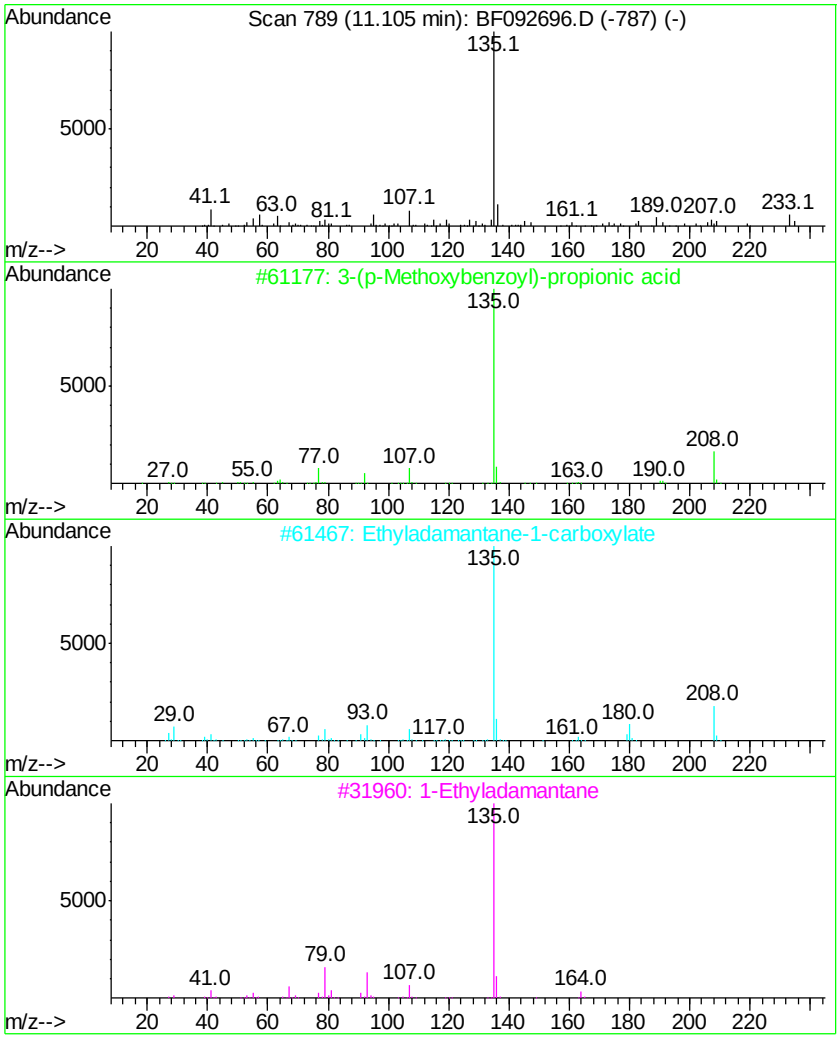
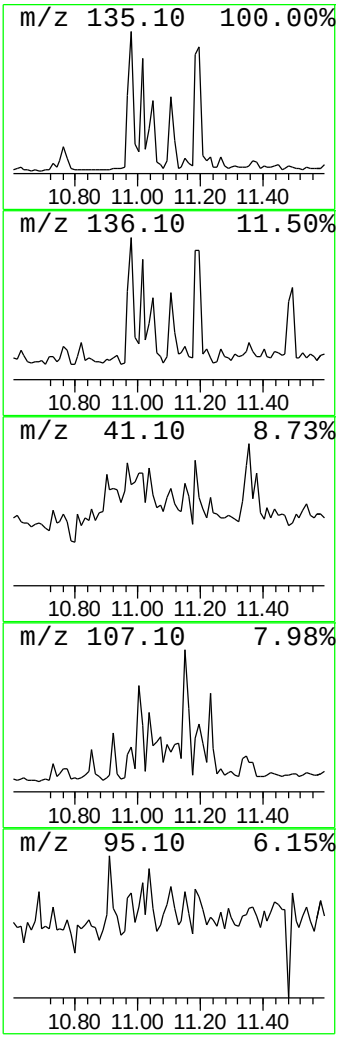
Peak Number 14 3-(p-Methoxybenzoyl)-propio... Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.10	2.56 ng	199401	Phenanthrene-d10	11.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-(p-Methoxybenzoyl)-propionic acid	208	C11H12O4	003153-44-4	72
2	Ethyladamantane-1-carboxylate	208	C13H20O2	002094-73-7	64
3	1-Ethyladamantane	164	C12H20	000770-69-4	64
4	3-Methyl-4-piperonyl-5-isoxazolone	233	C12H11NO4	014731-85-2	64
5	1,3,5-Tri-O-anisoyl-.alpha.-d-ri...	552	C29H28O11	1000129-91-9	64





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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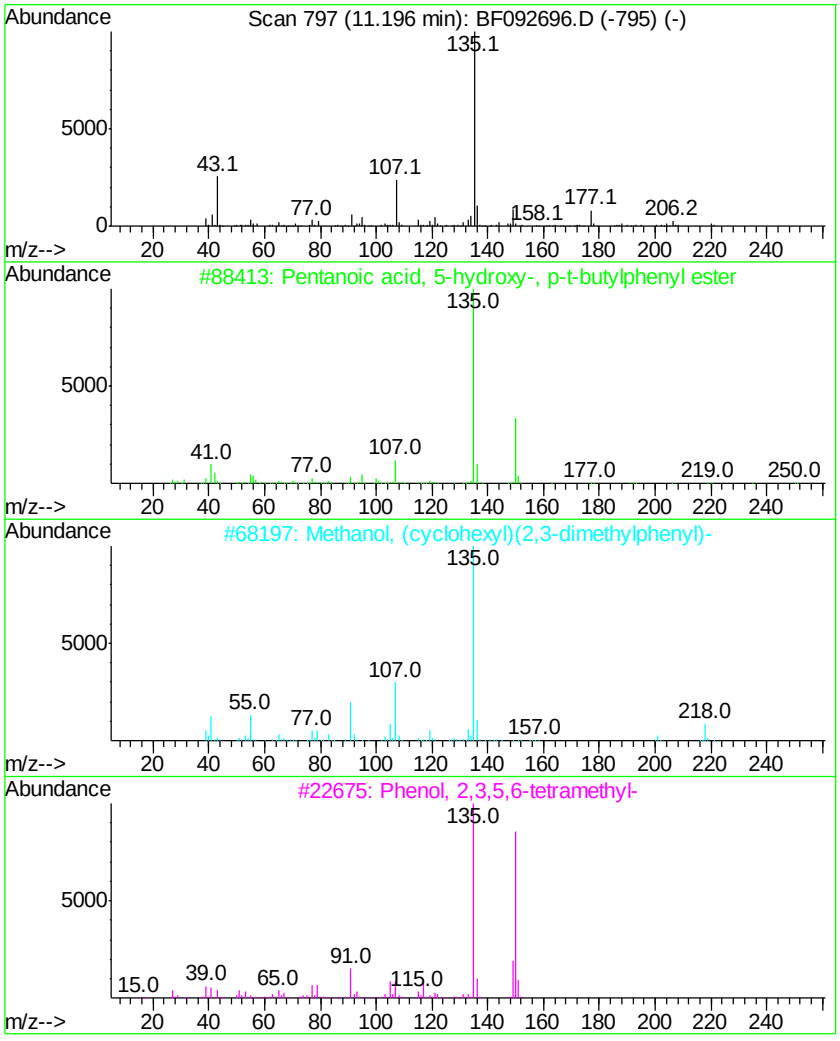
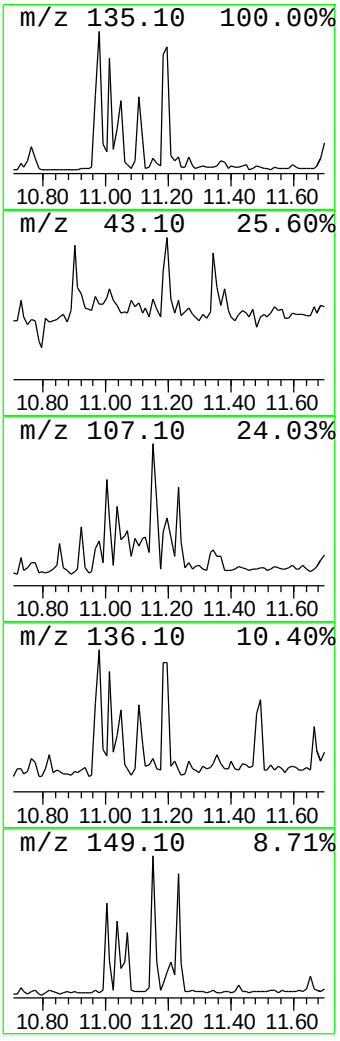
Peak Number 15 Pentanoic acid, 5-hydroxy-,... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.20	3.25 ng	253658	Phenanthrene-d10	11.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentanoic acid, 5-hydroxy-, p-t-...	250	C15H22O3	166273-37-6	64
2	Methanol, (cyclohexyl)(2,3-dimet...	218	C15H22O	349498-47-1	64
3	Phenol, 2,3,5,6-tetramethyl-	150	C10H14O	000527-35-5	59
4	Phenol, 4-(1,1,3,3-tetramethylbu...	206	C14H22O	000140-66-9	59
5	Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	56





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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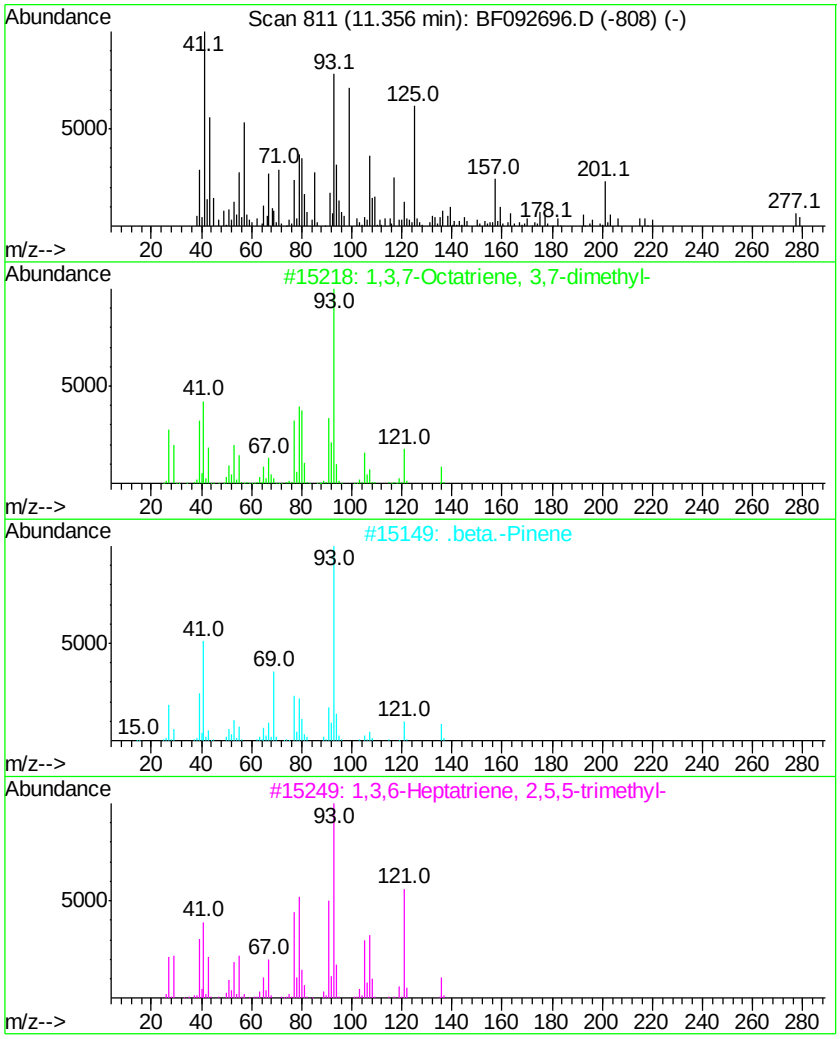
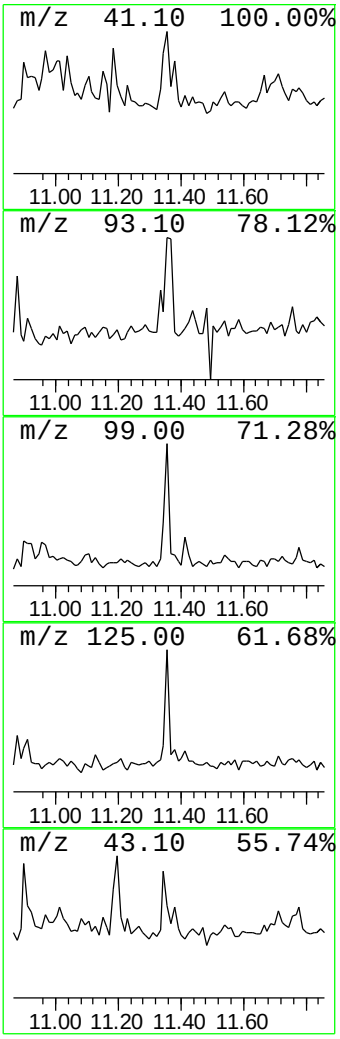
Peak Number 16 unknown11.36 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.36	2.81 ng	219370	Phenanthrene-d10	11.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,7-Octatriene, 3,7-dimethyl-	136	C10H16	000502-99-8	25
2	.beta.-Pinene	136	C10H16	000127-91-3	18
3	1,3,6-Heptatriene, 2,5,5-trimethyl-	136	C10H16	029548-02-5	18
4	Bicyclo[3.1.0]hexane, 4-methylen...	136	C10H16	003387-41-5	18
5	Cyclohexanemethanol, 4-methylene-	126	C8H14O	001004-24-6	18





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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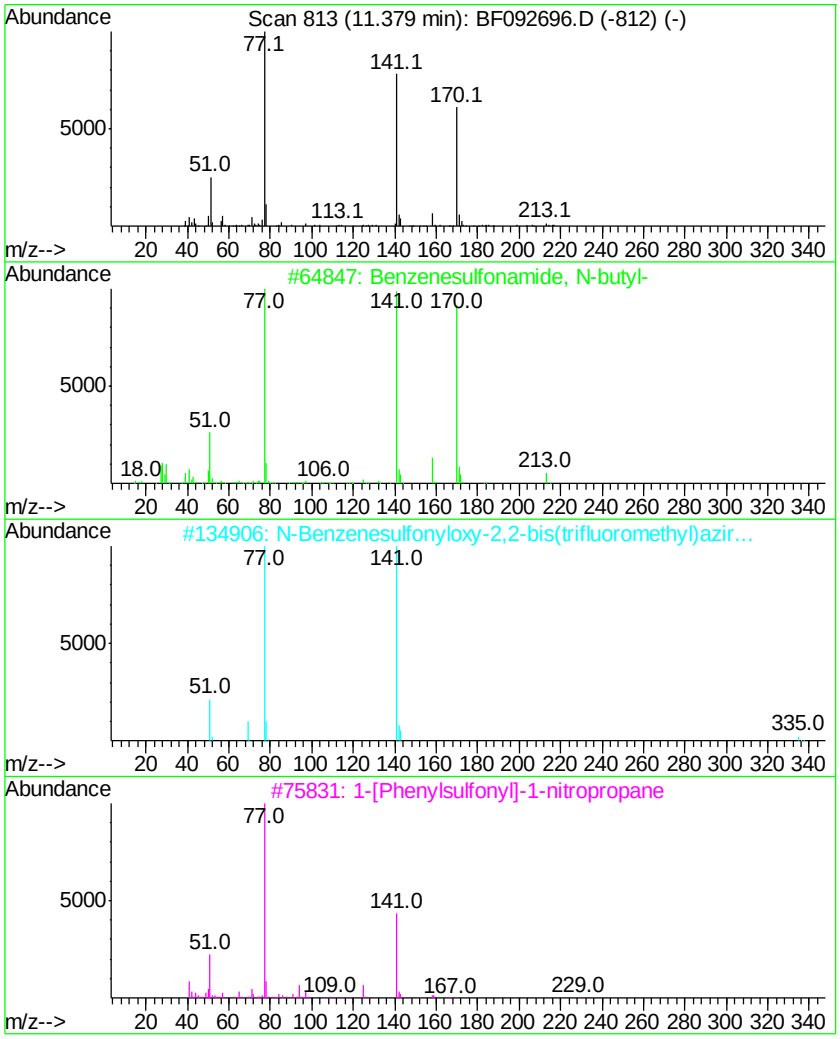
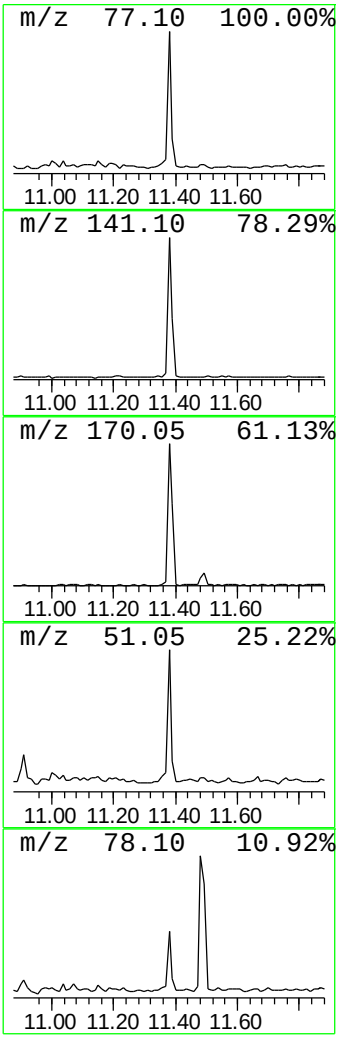
Peak Number 17 Benzenesulfonamide, N-butyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.38	2.93 ng	228801	Phenanthrene-d10	11.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenesulfonamide, N-butyl-	213	C10H15NO2S	003622-84-2	91
2	N-Benzenesulfonyloxy-2,2-bis(tri...	335	C10H7F6NO3S	055734-41-3	59
3	1-[Phenylsulfonyl]-1-nitropropane	229	C9H11NO4S	021272-84-4	50
4	N,N-Dichlorobenzenesulfonamide	225	C6H5Cl2NO2S	000473-29-0	50
5	p-Chloromandelic acid	186	C8H7ClO3	000492-86-4	45





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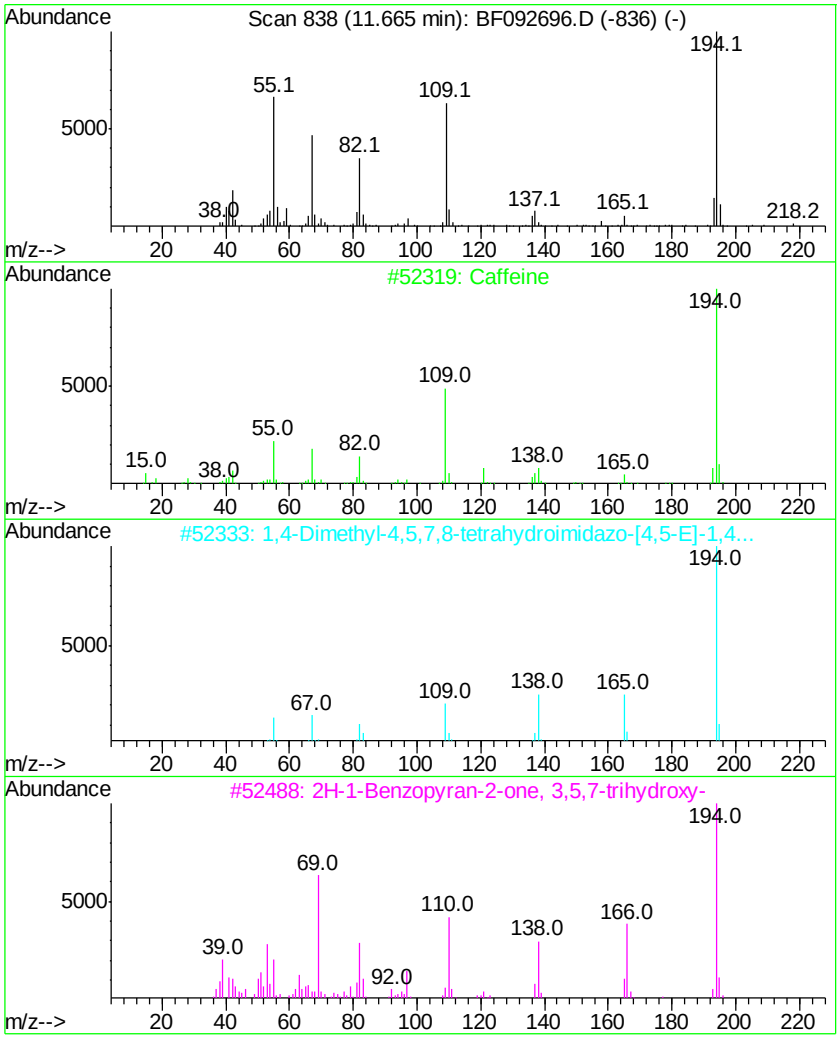
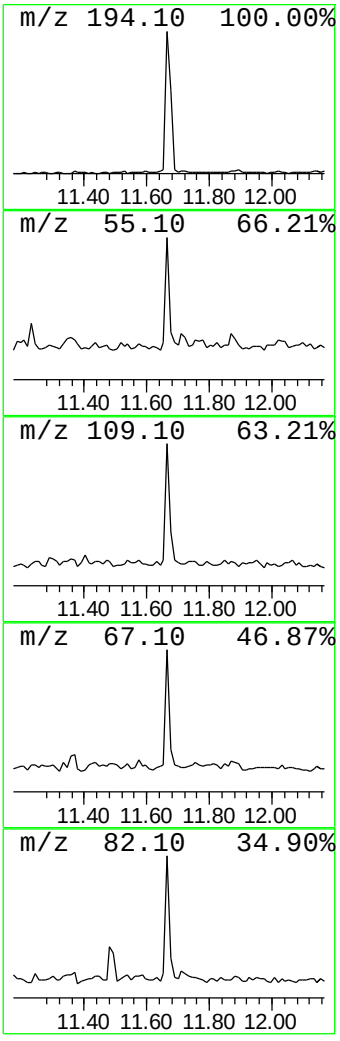
Peak Number 18 Caffeine Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.67	2.79 ng	217464	Phenanthrene-d10	11.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Caffeine	194	C8H10N4O2	000058-08-2	94
2	1,4-Dimethyl-4,5,7,8-tetrahydroi...	194	C8H10N4O2	130063-15-9	47
3	2H-1-Benzopyran-2-one, 3,5,7-tri...	194	C9H6O5	022065-07-2	43
4	1H-Benzimidazole, 2-phenyl-	194	C13H10N2	000716-79-0	38
5	2-Acetylpyridine thiosemicarbazone	194	C8H10N4S	006839-90-3	35





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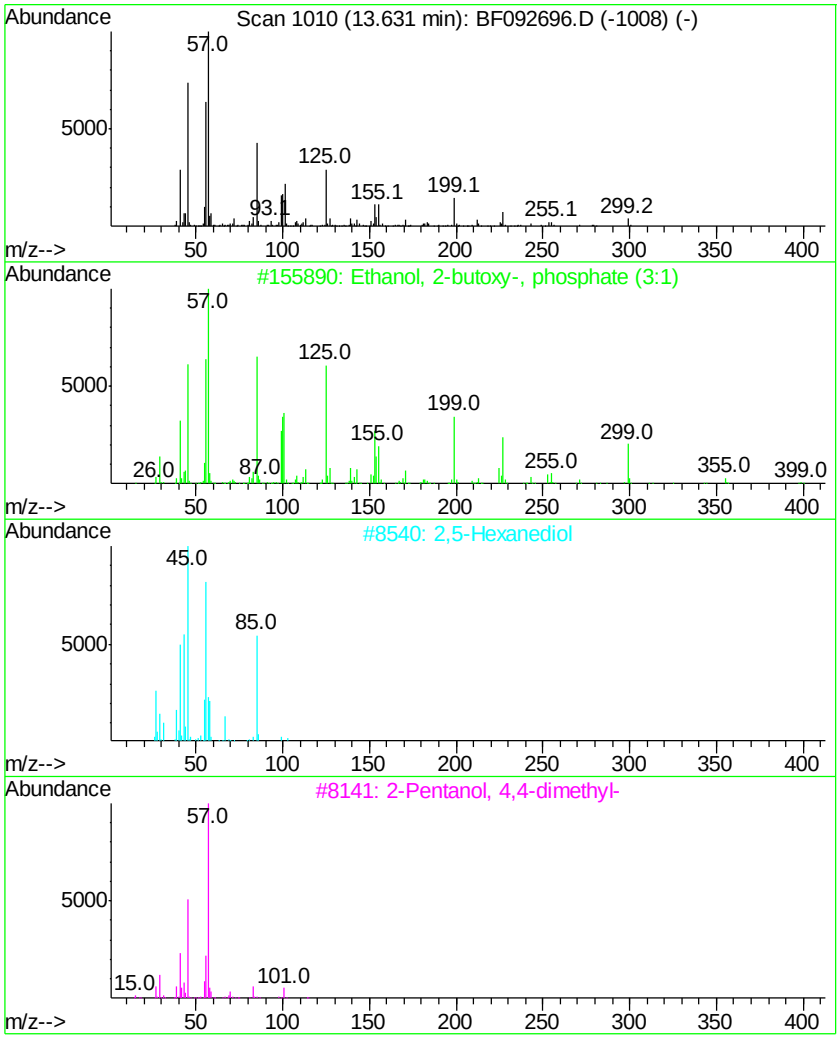
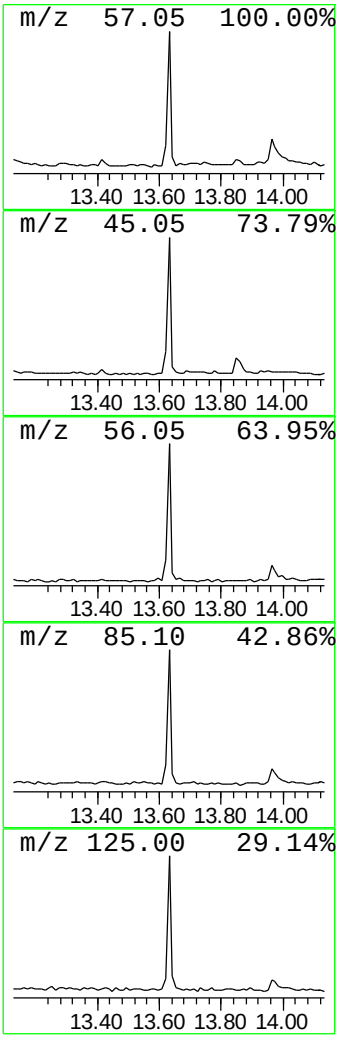
Peak Number 19 Ethanol, 2-butoxy-, phospha... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.63	4.74 ng	281864	Chrysene-d12	14.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-butoxy-, phosphate (3:1)	398	C18H39O7P	000078-51-3	91
2	2,5-Hexanediol	118	C6H14O2	002935-44-6	50
3	2-Pentanol, 4,4-dimethyl-	116	C7H16O	006144-93-0	35
4	1,5-Hexanediol	118	C6H14O2	000928-40-5	32
5	Formic acid, 1-methylpropyl ester	102	C5H10O2	000589-40-2	27





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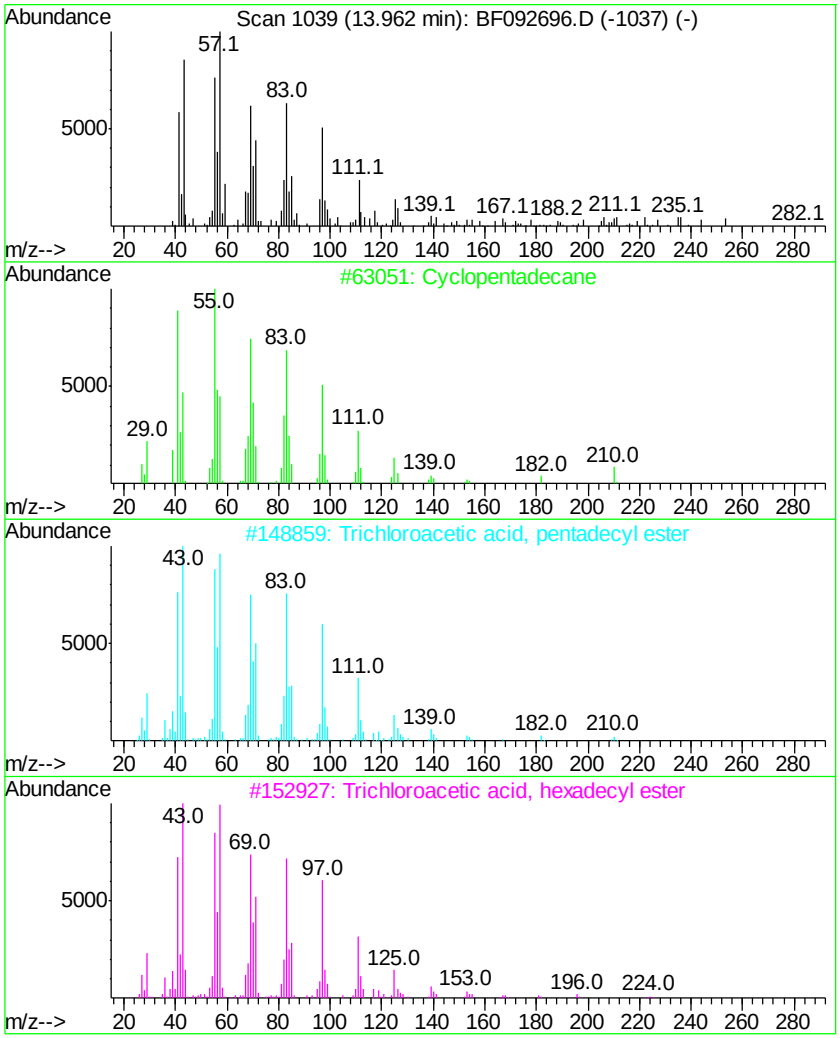
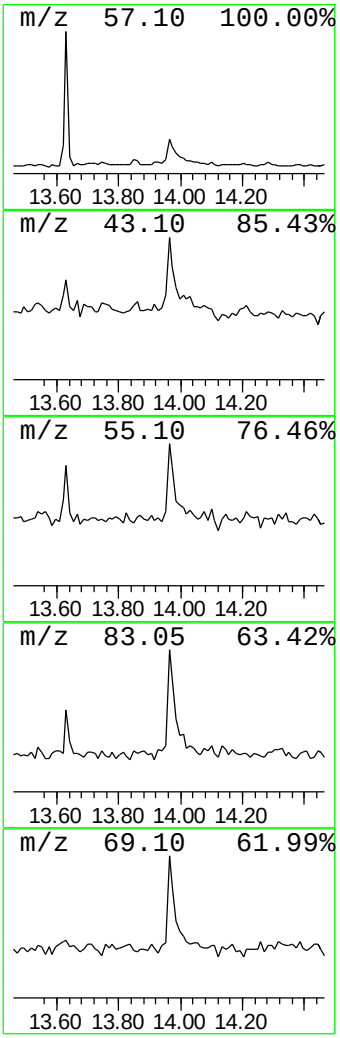
Peak Number 20 Cyclopentadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.96	3.22 ng	191329	Chrysene-d12	14.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentadecane	210	C15H30	000295-48-7	97
2	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	93
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	93
4	1-Pentadecanethiol	244	C15H32S	025276-70-4	90
5	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	89





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF013117\
Data File : BF092696.D
Acq On : 31 Jan 2017 22:14
Operator : SJ/MA
Sample : I1596-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-19

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.13	17.0	ng	885348	1	6.94	1041840	20.0
unknown6.72	6.72	67.8	ng	3529370	1	6.94	1041840	20.0
3-Heptanol, 3,6-d...	6.80	2.5	ng	127778	1	6.94	1041840	20.0
1-Propanol, 2-(2-...	7.86	5.3	ng	357365	2	8.24	1341110	20.0
2-Butanol, 3,3'-o...	7.88	5.1	ng	343534	2	8.24	1341110	20.0
5-Ethyl-3-methylh...	7.97	3.3	ng	218000	2	8.24	1341110	20.0
2,4-Diethyl-6-met...	8.48	3.7	ng	247544	2	8.24	1341110	20.0
Ethyl citrate	10.67	3.2	ng	256371	3	10.00	1613770	20.0
2(3H)-Benzothiazo...	10.91	5.0	ng	390080	4	11.49	1560350	20.0
Phenol, 4-(1,1,3,...	10.98	2.5	ng	196709	4	11.49	1560350	20.0
unknown11.00	11.00	2.9	ng	223400	4	11.49	1560350	20.0
unknown11.04	11.04	2.6	ng	201843	4	11.49	1560350	20.0
3-(p-Methoxybenzo...	11.10	2.6	ng	199401	4	11.49	1560350	20.0
Pentanoic acid, 5...	11.20	3.3	ng	253658	4	11.49	1560350	20.0
unknown11.36	11.36	2.8	ng	219370	4	11.49	1560350	20.0
Benzenesulfonamid...	11.38	2.9	ng	228801	4	11.49	1560350	20.0
Caffeine	11.67	2.8	ng	217464	4	11.49	1560350	20.0
Ethanol, 2-butoxy...	13.63	4.7	ng	281864	5	14.12	1189790	20.0
Cyclopentadecane	13.96	3.2	ng	191329	5	14.12	1189790	20.0