LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF031017\
Data File : BF093547.D
Acq On : 11 Mar 2017 3:05
Operator : SJ/MA
Sample : I2198-07
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-13

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-BF030717.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	4.893	261	263	275	rBV	137829	286519	6.09%	0.683%
2	5.339	301	302	314	rBV	1418728	2392558	50.85%	5.704%
3	6.424	394	397	403	rBV	648688	1502391	31.93%	3.582%
4	6.516	403	405	410	rVB	3390327	4001933	85.05%	9.541%
5	6.733	422	424	427	rBV	797007	1178357	25.04%	2.809%
6	6.893	436	438	441	rBV	3777595	3501302	74.41%	8.348%
7	6.962	442	444	448	rVB	63261	103578	2.20%	0.247%
8	7.087	453	455	458	rVB	76949	81952	1.74%	0.195%
9	7.259	469	470	472	rVB	96404	75763	1.61%	0.181%
10	7.316	472	475	483	rBV	3446414	3669188	77.98%	8.748%
11	7.442	483	486	490	rVB4	48222	121170	2.58%	0.289%
12	7.567	494	497	498	rBV2	71734	87777	1.87%	0.209%
13	7.602	498	500	504	rVB2	86216	121641	2.59%	0.290%
14	7.705	506	509	511	rBV3	31505	53265	1.13%	0.127%
15	7.750	511	513	515	rBV2	37774	62217	1.32%	0.148%
16	7.830	518	520	523	rBV2	33558	76503	1.63%	0.182%
17	7.967	526	532	535	rBV3	126400	296265	6.30%	0.706%
18	8.025	535	537	545	rVB	1703271	1903688	40.46%	4.539%
19	8.139	545	547	549	rBV3	51711	100483	2.14%	0.240%
20	8.185	549	551	552	rBV2	61336	82382	1.75%	0.196%
21	8.265	555	558	560	rBV3	97261	202689	4.31%	0.483%
22	8.402	567	570	573	rBV5	83860	238609	5.07%	0.569%
23	8.459	573	575	577	rVB	65916	67064	1.43%	0.160%
24	8.505	577	579	582	rBV3	173722	223798	4.76%	0.534%
25	8.550	582	583	585	rBV	100812	89975	1.91%	0.215%
26	8.642	589	591	592	rVB	82110	61606	1.31%	0.147%
27	8.699	592	596	597	rVB3	40937	98322	2.09%	0.234%
28	8.745	597	600	601	rBV3	66602	143408	3.05%	0.342%
29	8.768	601	602	606	rVB2	95545	141690	3.01%	0.338%
30	8.836	606	608	609	rBV2	64048	88165	1.87%	0.210%
31	8.916	612	615	617	rVB4	123097	200235	4.26%	0.477%
32	9.019	619	624	625	rBV3	98720	261830	5.56%	0.624%
33	9.053	625	627	628	rVV	224063	183333	3.90%	0.437%
34	9.099	628	631	634	rVB	4531668	4705124	100.00%	11.218%

LSC Area Percent Report

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Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-13

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-BF030717.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	9.225	640	642	643	rBV	85709	83457	1.77%	0.199%
36	9.282	646	647	649	rVV2	147036	170003	3.61%	0.405%
37	9.396	653	657	659	rBV3	280478	623655	13.25%	1.487%
38	9.431	659	660	661	rVV	179175	163708	3.48%	0.390%
39	9.499	665	666	669	rVV2	163202	239688	5.09%	0.571%
40	9.602	672	675	676	rBV3	65161	144645	3.07%	0.345%
41	9.773	688	690	696	rBV	1821066	1939084	41.21%	4.623%
42	10.162	720	724	726	rBV4	106129	216446	4.60%	0.516%
43	10.539	755	757	758	rBV	157133	140464	2.99%	0.335%
44	10.573	758	760	763	rVV	2405123	2577052	54.77%	6.144%
45	10.699	768	771	773	rBV2	210822	310065	6.59%	0.739%
46	11.019	797	799	800	rBV2	99721	114297	2.43%	0.273%
47	11.134	806	809	811	rVB2	252965	360125	7.65%	0.859%
48	11.259	818	820	823	rBV	1593314	1589603	33.78%	3.790%
49	11.808	866	868	872	rVB3	149194	251351	5.34%	0.599%
50	12.848	956	959	961	rBV	4070951	4241864	90.15%	10.113%
51	13.900	1049	1051	1054	rBV	1287504	1227644	26.09%	2.927%
52	15.305	1171	1174	1187	rVB	758267	1144725	24.33%	2.729%

Sum of corrected areas: 41942656

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Instrument : BNA_F
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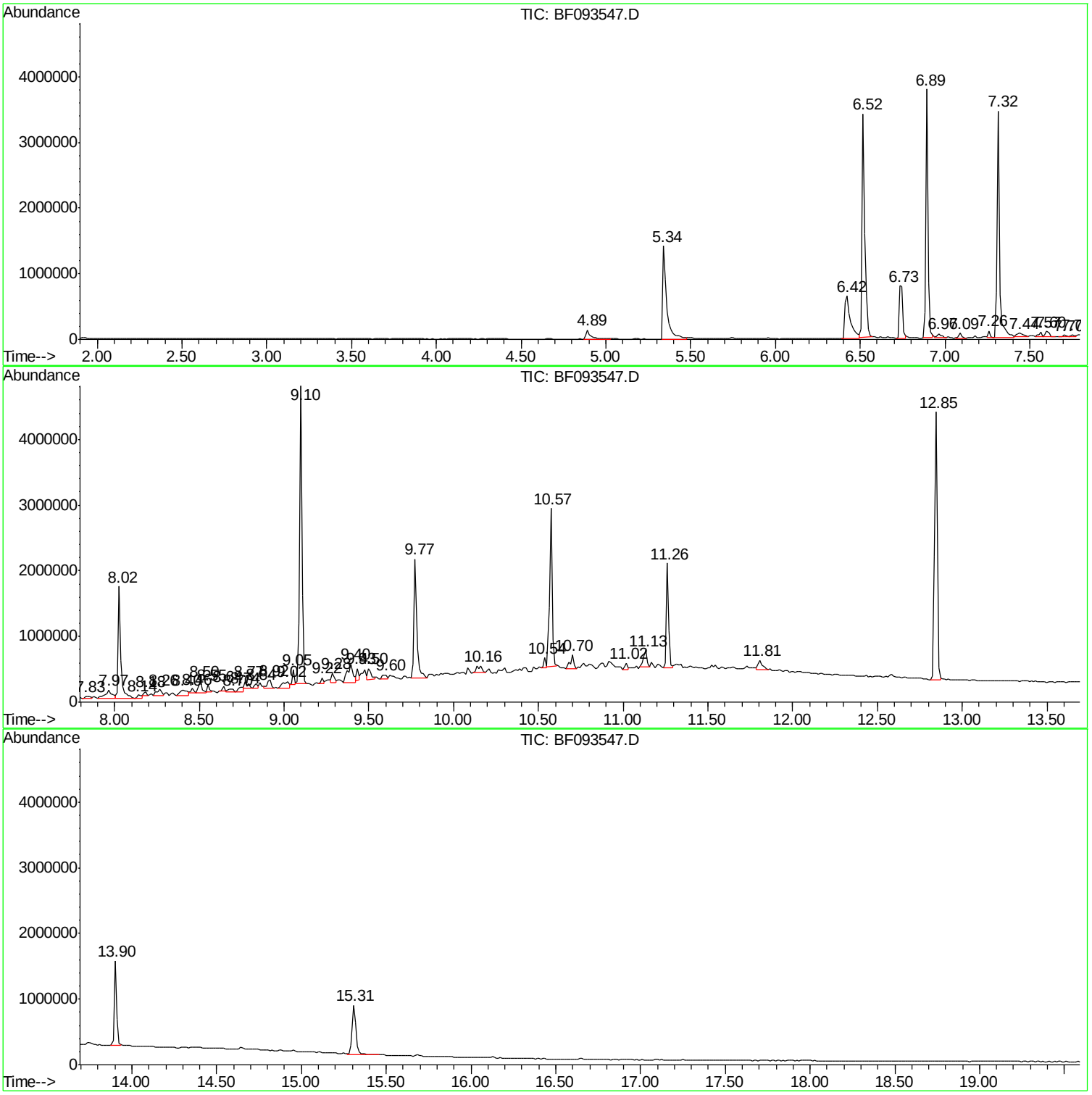
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.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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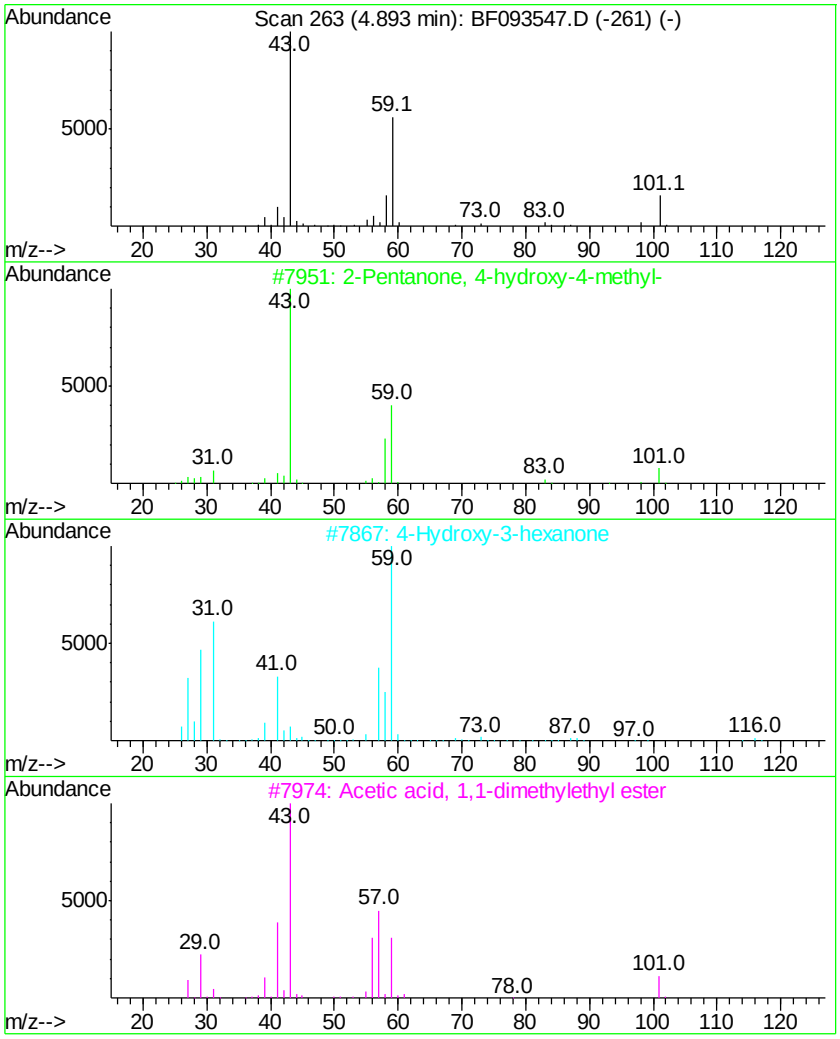
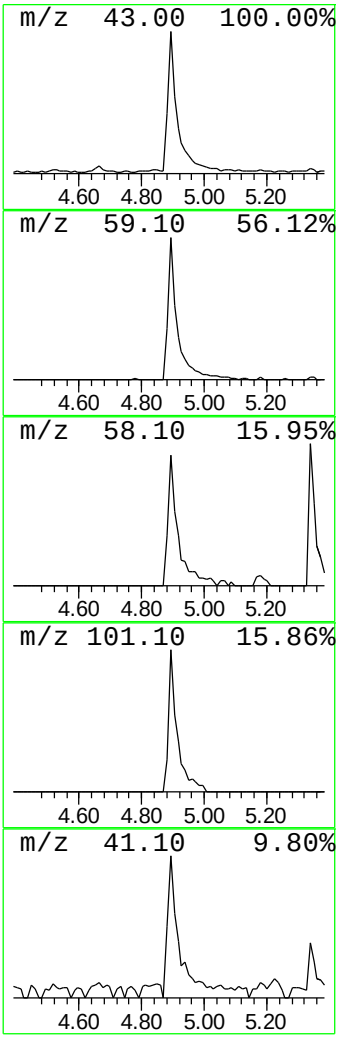
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.89	4.86 ng	286519	1,4-Dichlorobenzene-d4	6.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	37
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28





Data Path : Z:\HPCHEM1\BNA F\DATA\BF031017\
Data File : BF093547.D
Acq On : 11 Mar 2017 3:05
Operator : SJ/MA
Sample : I2198-07
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-13

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

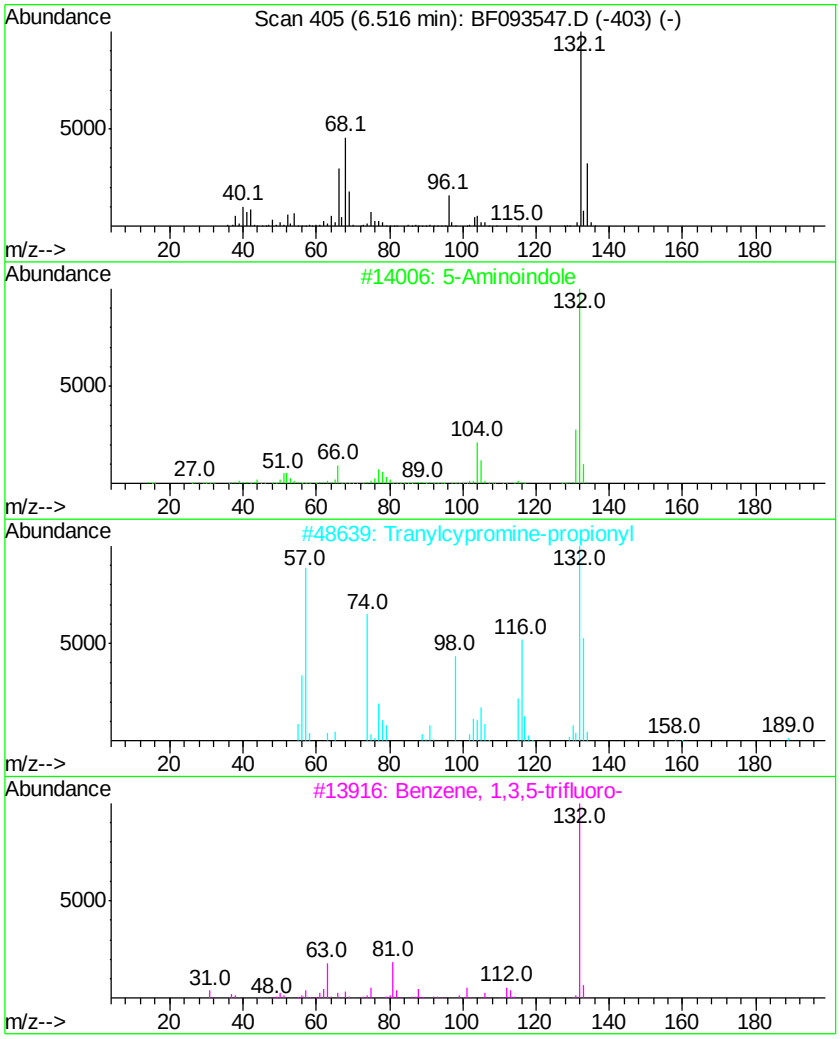
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

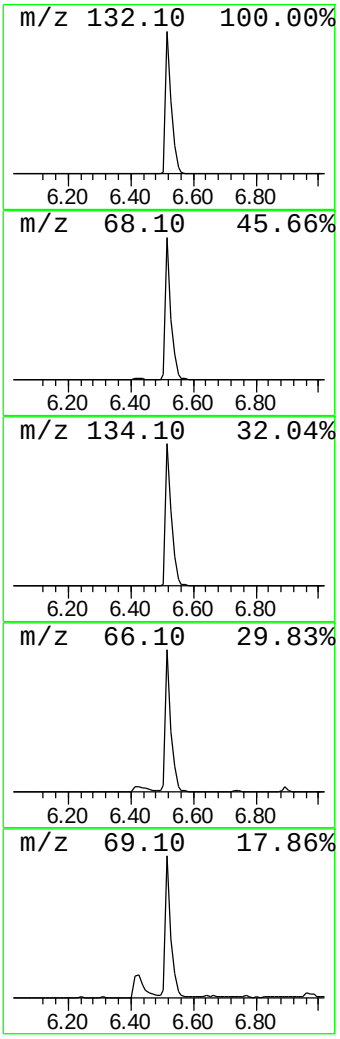
****

Peak Number 2 unknown6.52 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.52	67.92 ng	4001930	1,4-Dichlorobenzene-d4	6.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Aminoindole	132	C8H8N2	005192-03-0	12
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF031017\
Data File : BF093547.D
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Operator : SJ/MA
Sample : I2198-07
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-13

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.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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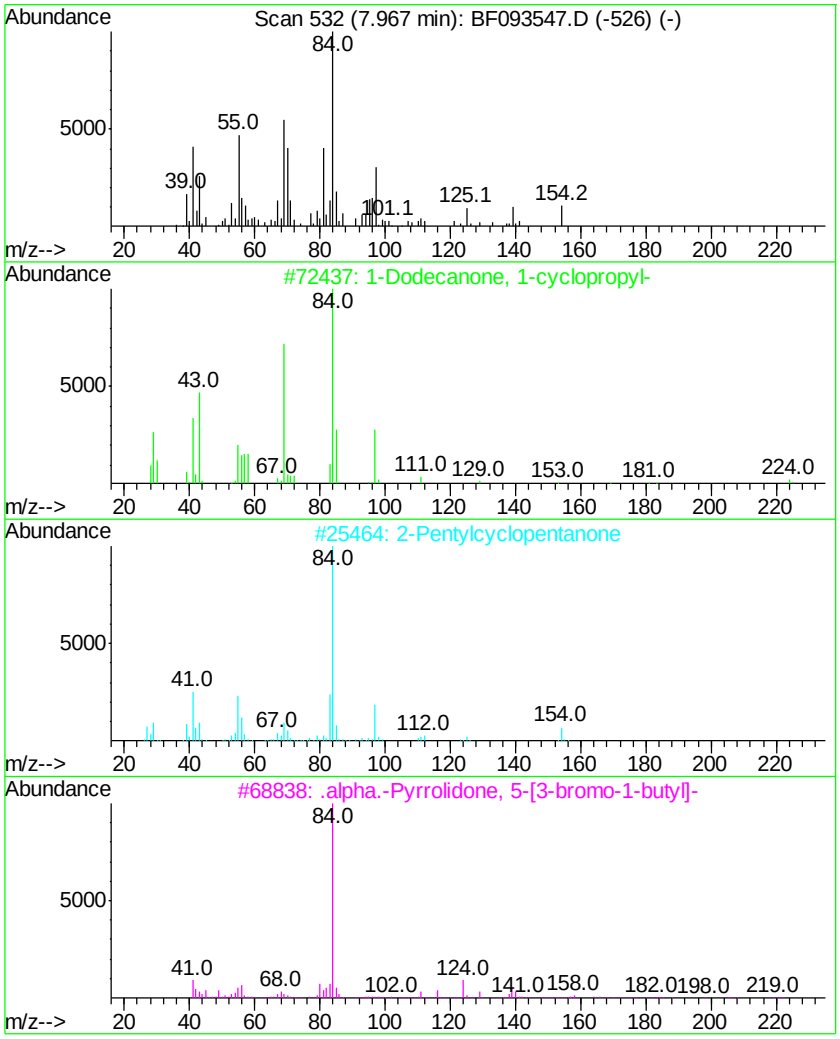
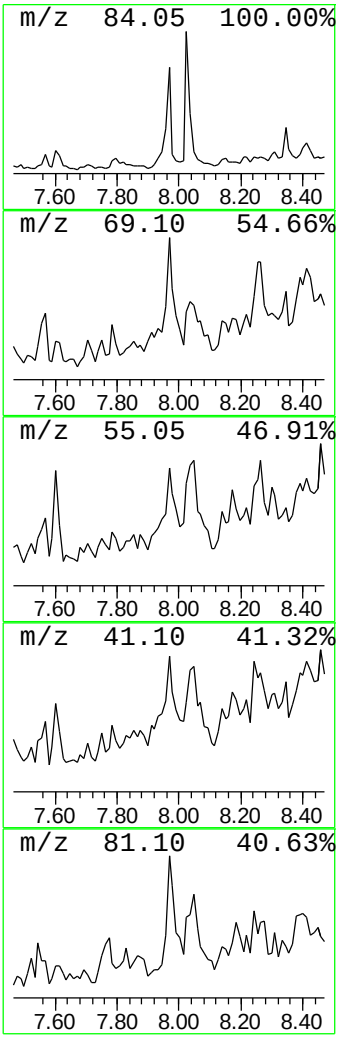
Peak Number 4 unknown7.97 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.97	3.11 ng	296265	Naphthalene-d8	8.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Dodecanone, 1-cyclopropyl-	224	C15H28O	019873-44-0	37
2	2-Pentylcyclopentanone	154	C10H18O	1000191-05-3	37
3	.alpha.-Pyrrolidone, 5-[3-bromo-...	219	C8H14BrNO	1000125-95-7	35
4	1-Methoxy-4,4-dimethyl-cyclohex-...	140	C9H16O	073741-65-8	32
5	Perdeuterobenzene	84	C6D6	001076-43-3	27





Library Search Compound Report

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Sample : I2198-07
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-13

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

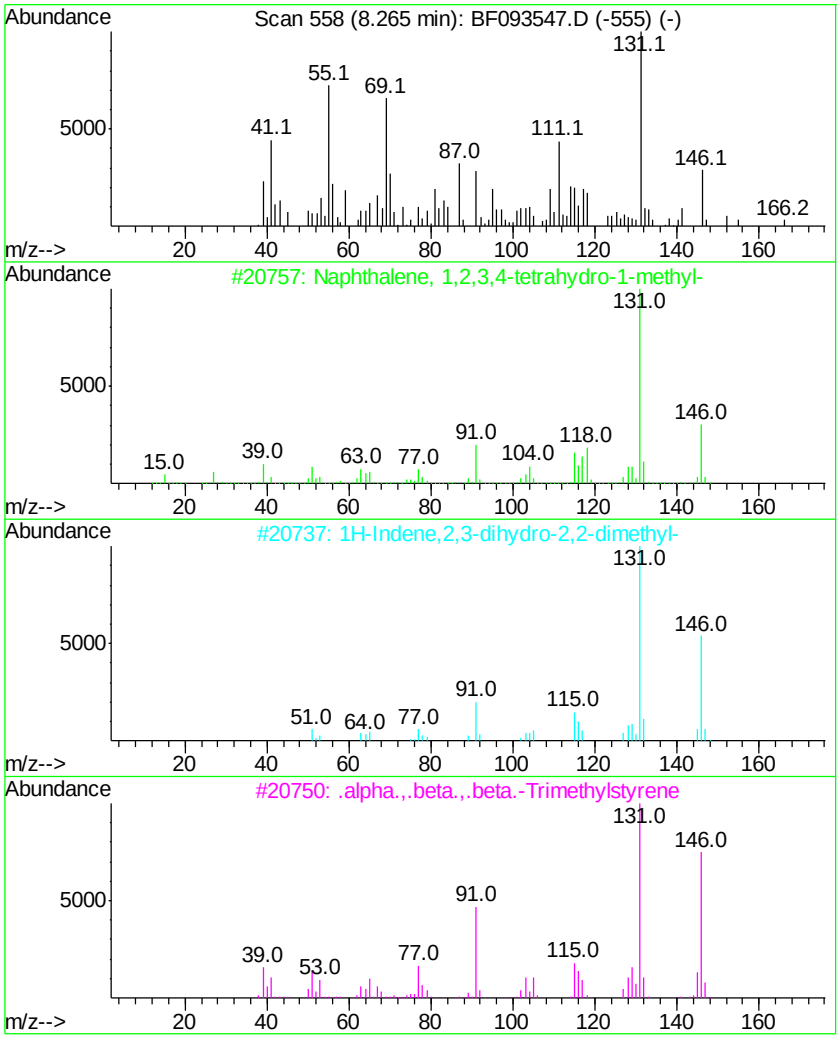
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

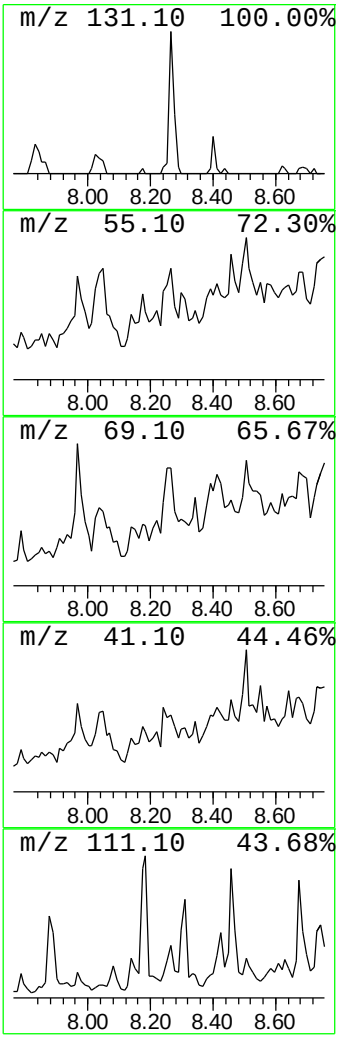
****

Peak Number 5 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.26	2.13 ng	202689	Naphthalene-d8	8.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001559-81-5	50
2	1H-Indene,2,3-dihydro-2,2-dimethyl-	146	C11H14	020836-11-7	46
3	.alpha.,.beta.,.beta.-Trimethyls...	146	C11H14	000769-57-3	43
4	Benzene, (3-methyl-2-butenyl)-	146	C11H14	004489-84-3	41
5	Benzene, 1-methyl-4-(1-methyl-2-...	146	C11H14	097664-18-1	38





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Sample : I2198-07
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Instrument : BNA_F
ClientSampleId : W-13

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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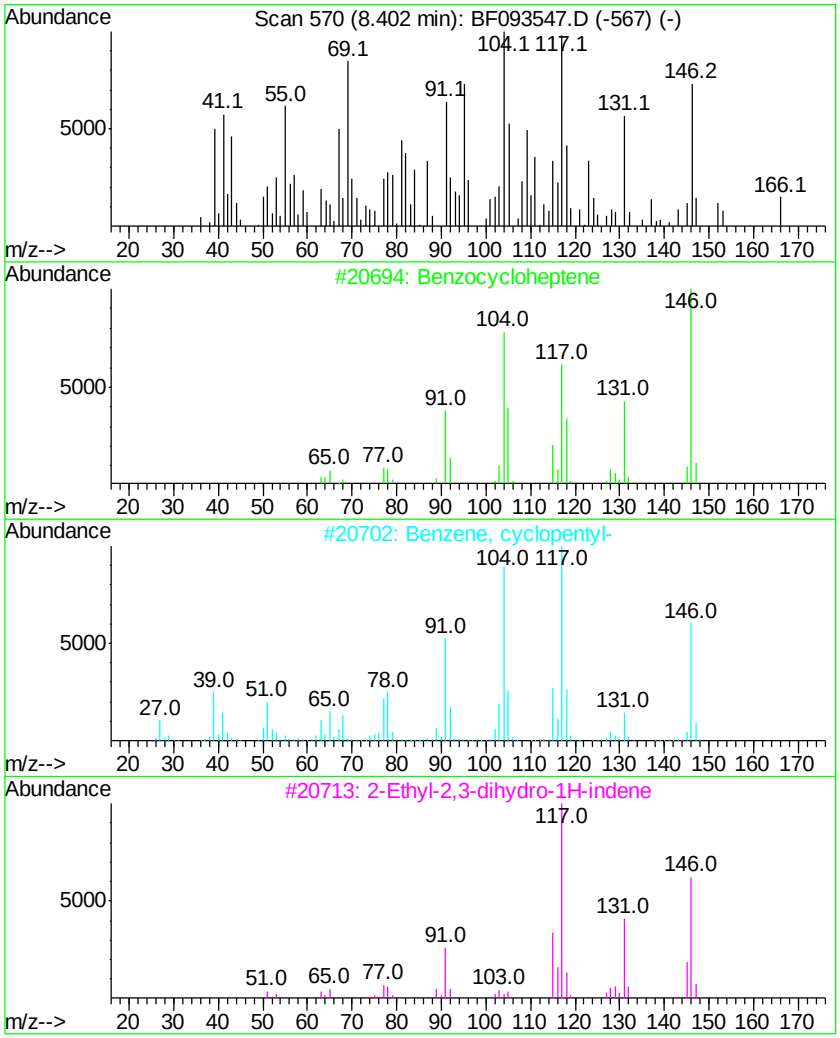
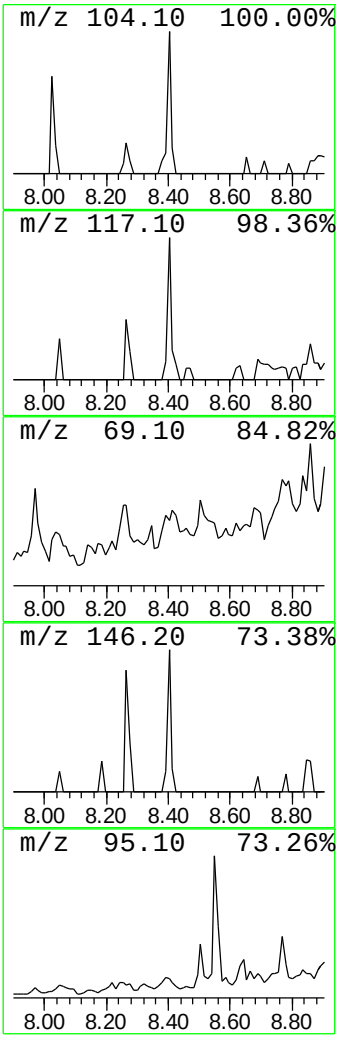
Peak Number 6 Benzocycloheptene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.40	2.51 ng	238609	Naphthalene-d8	8.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzocycloheptene	146	C11H14	001075-16-7	90
2	Benzene, cyclopentyl-	146	C11H14	000700-88-9	89
3	2-Ethyl-2,3-dihydro-1H-indene	146	C11H14	056147-63-8	42
4	trans-1-Phenyl-1-pentene	146	C11H14	016002-93-0	38
5	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	35





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Sample : I2198-07
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-13

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.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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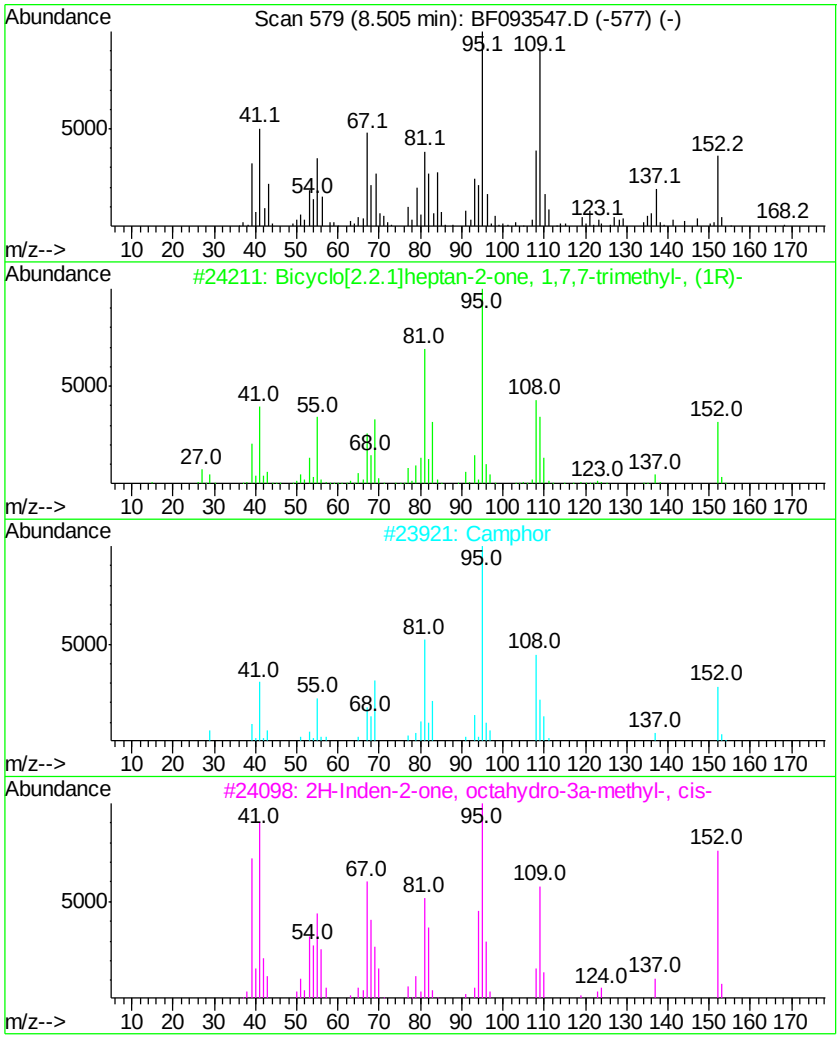
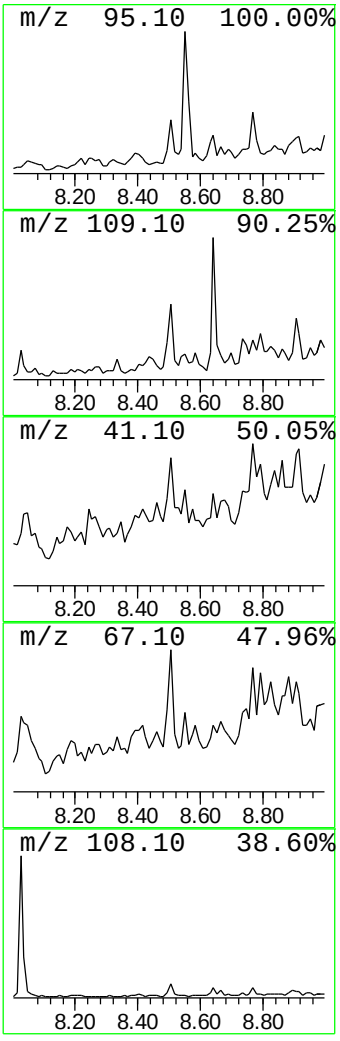
Peak Number 7 unknown8.50 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.50	2.35 ng	223798	Naphthalene-d8	8.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-49-3	49
2	Camphor	152	C10H16O	000076-22-2	43
3	2H-Inden-2-one, octahydro-3a-met...	152	C10H16O	013351-29-6	38
4	1-Adamantanol	152	C10H16O	000768-95-6	30
5	Bicyclo[3.1.0]hexane, 1,5-dimethyl-	110	C8H14	1000142-17-5	30





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

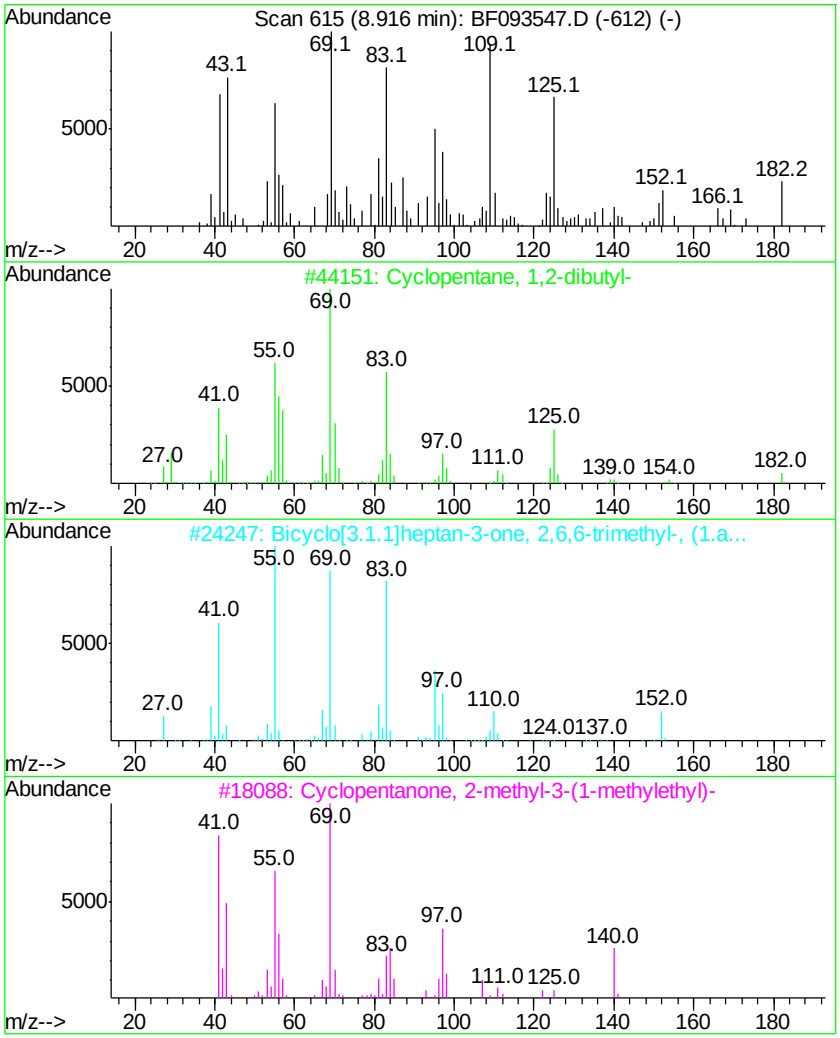
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

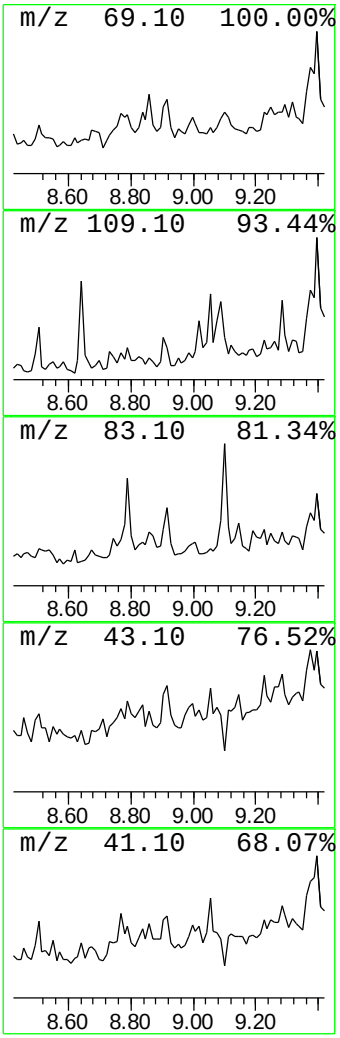
****

Peak Number 8 Cyclopentane, 1,2-dibutyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.92	2.07 ng	200235	Acenaphthene-d10	9.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, 1,2-dibutyl-	182	C13H26	062199-52-4	53
2	Bicyclo[3.1.1]heptan-3-one, 2,6,...	152	C10H16O	015358-88-0	43
3	Cyclopentanone, 2-methyl-3-(1-me...	140	C9H16O	054549-81-4	38
4	3-Octene, 2,2-dimethyl-	140	C10H20	086869-76-3	38
5	Cyclohexane, 1,1,3,5-tetramethyl...	140	C10H20	050876-32-9	35





Data Path : Z:\HPCHEM1\BNA F\DATA\BF031017\
Data File : BF093547.D
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Operator : SJ/MA
Sample : I2198-07
Misc :
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Instrument : BNA_F
ClientSampleId : W-13

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.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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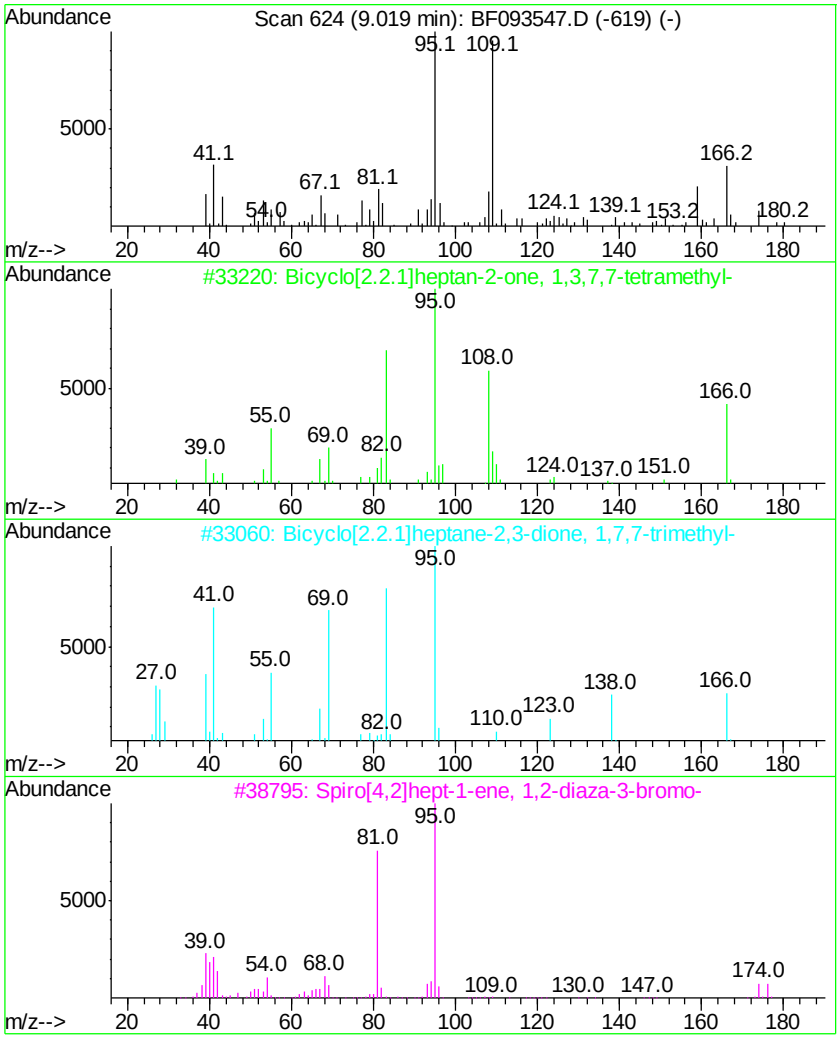
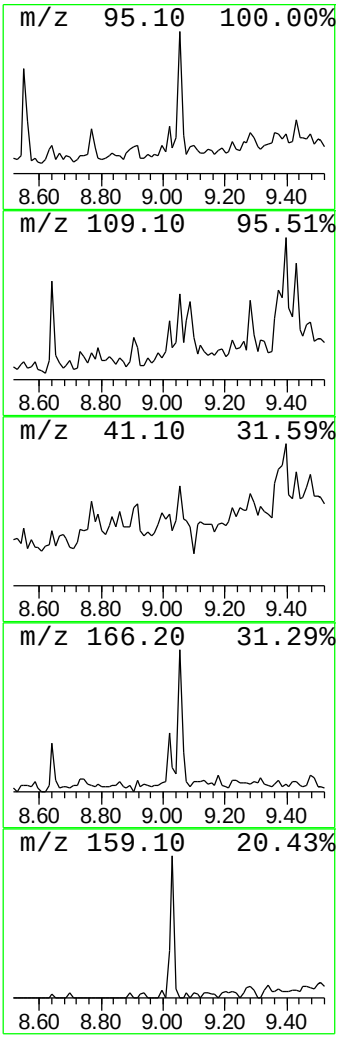
Peak Number 9 unknown9.02 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.02	2.70 ng	261830	Acenaphthene-d10	9.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[2.2.1]heptan-2-one, 1,3,...	166	C11H18O	005811-48-3	38
2	Bicyclo[2.2.1]heptane-2,3-dione,...	166	C10H14O2	000465-29-2	38
3	Spiro[4.2]hept-1-ene, 1,2-diaza-...	174	C5H7BrN2	211738-70-4	27
4	2-Cyclopentene-1-butanal, .gamma....	194	C13H22O	060714-25-2	27
5	Cyclohexanemethanol, 4-(1-methyl...	156	C10H20O	013828-37-0	27





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Data File : BF093547.D
Acq On : 11 Mar 2017 3:05
Operator : SJ/MA
Sample : I2198-07
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-13

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.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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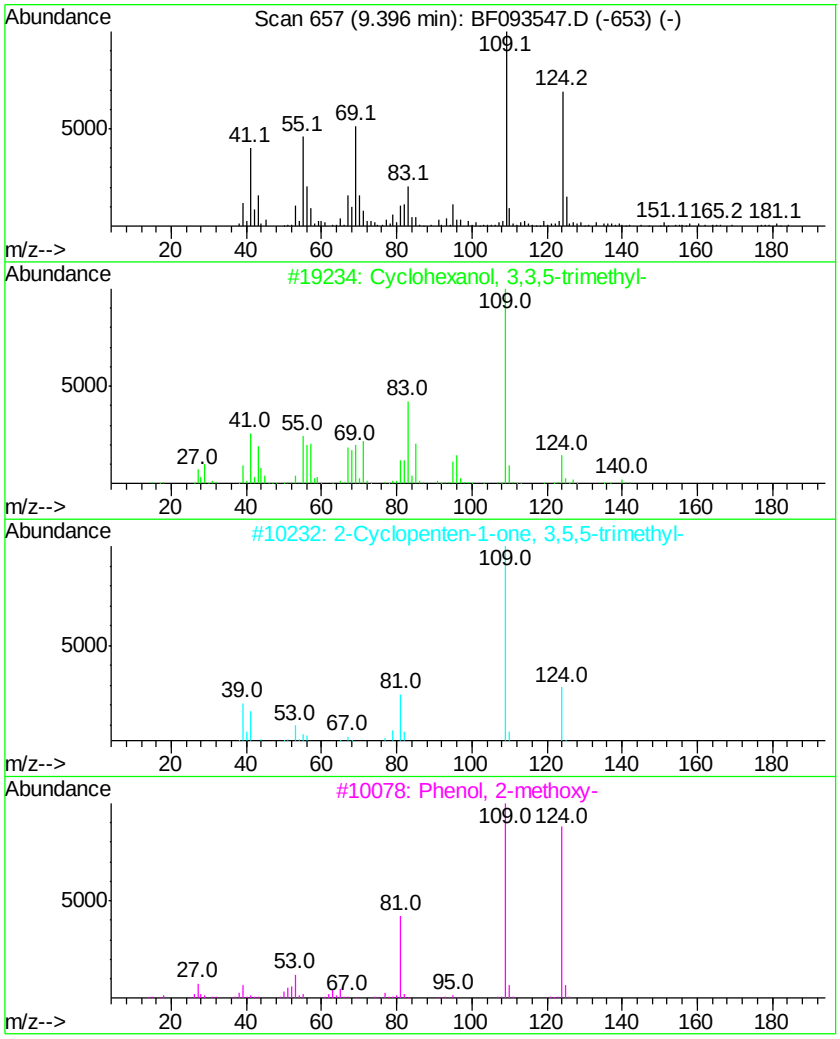
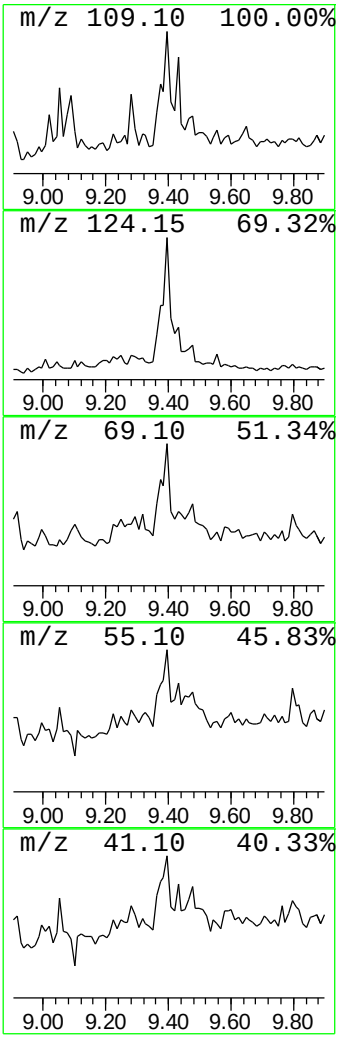
Peak Number 10 Cyclohexanol, 3,3,5-trimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.40	6.43 ng	623655	Acenaphthene-d10	9.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanol, 3,3,5-trimethyl-	142	C9H18O	000116-02-9	58
2	2-Cyclopenten-1-one, 3,5,5-trime...	124	C8H12O	024156-95-4	53
3	Phenol, 2-methoxy-	124	C7H8O2	000090-05-1	50
4	2-Cyclopenten-1-one, 3,4,4-trime...	124	C8H12O	030434-65-2	50
5	Mequinol	124	C7H8O2	000150-76-5	50





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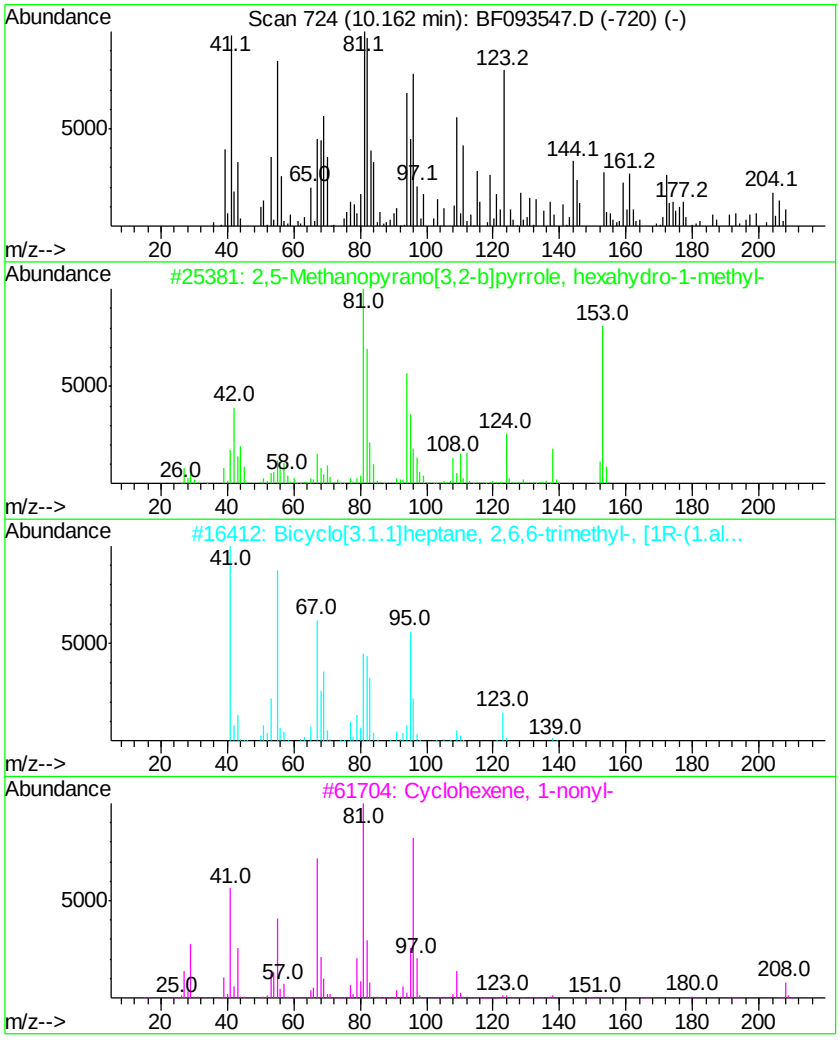
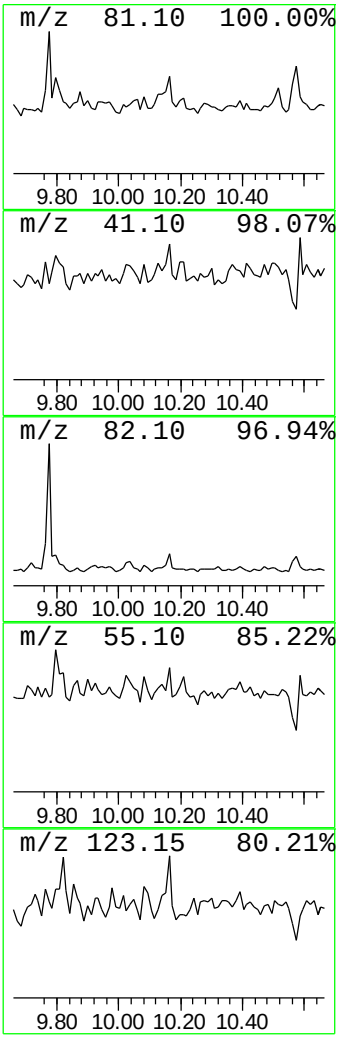
Peak Number 11 unknown10.16 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.16	2.23 ng	216446	Acenaphthene-d10	9.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5-Methanopyrano[3,2-b]pyrrole,...	153	C9H15NO	1000188-76-3	38
2	Bicyclo[3.1.1]heptane, 2,6,6-tri...	138	C10H18	004795-86-2	27
3	Cyclohexene, 1-nonyl-	208	C15H28	015232-88-9	27
4	4H-1,3-Benzodioxin-4-one, hexahy...	170	C9H14O3	124899-15-6	25
5	Cyclohexene, 3-nonyl-	208	C15H28	015232-79-8	25





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Instrument : BNA_F
ClientSampleId : W-13

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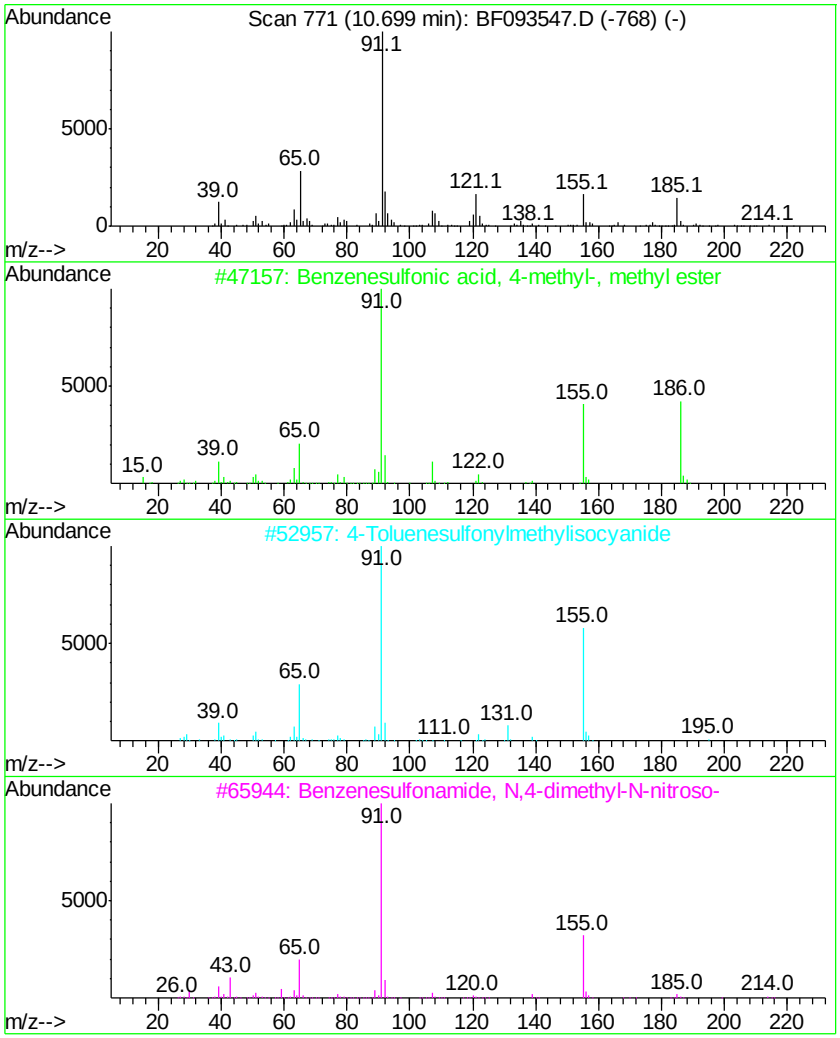
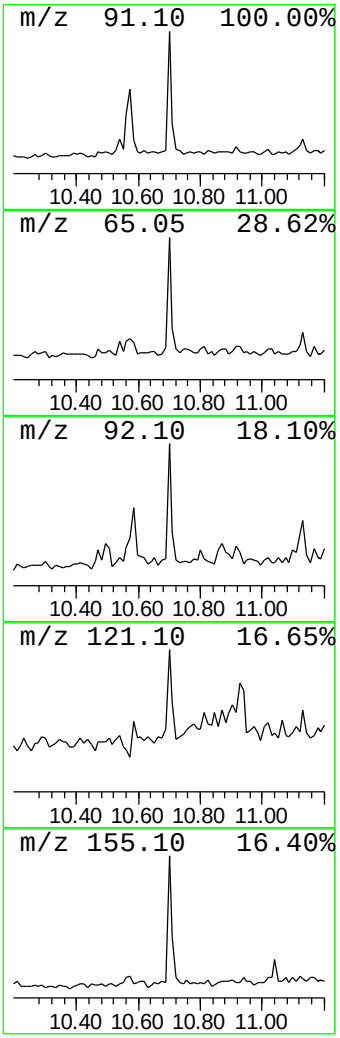
Peak Number 12 Benzenesulfonic acid, 4-met... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.70	3.90 ng	310065	Phenanthrene-d10	11.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenesulfonic acid, 4-methyl-,...	186	C8H10O3S	000080-48-8	68
2	4-Toluenesulfonylmethylisocyanide	195	C9H9NO2S	036635-61-7	53
3	Benzenesulfonamide, N,4-dimethyl...	214	C8H10N2O3S	000080-11-5	50
4	Benzenesulfonamide, N,4-dimethyl-	185	C8H11NO2S	000640-61-9	49
5	Toluene-4-sulfonic acid, 2-benzy...	366	C18H22O6S	118653-93-3	43





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ClientSampleId : W-13

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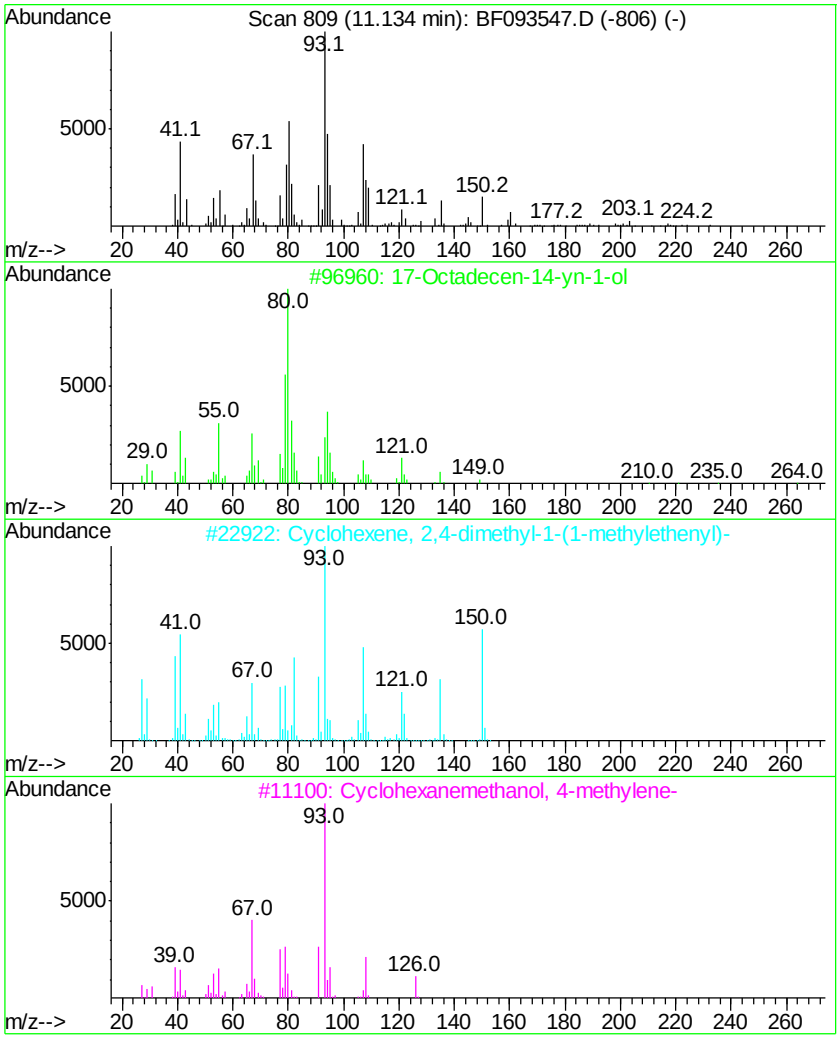
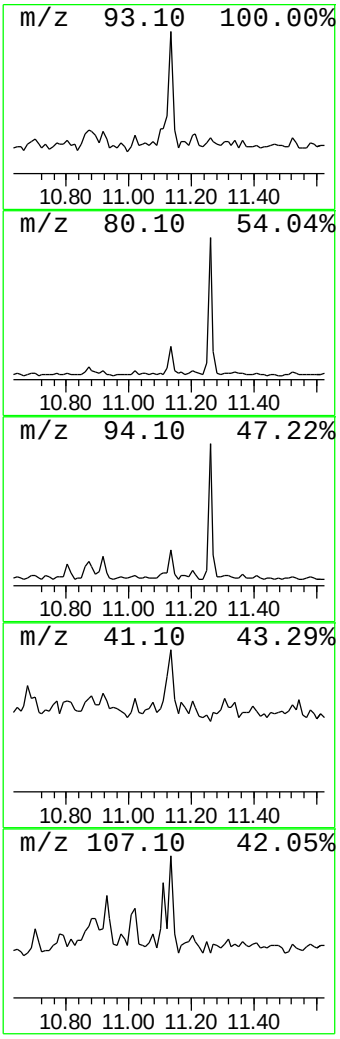
Peak Number 13 unknown11.13 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.13	4.53 ng	360125	Phenanthrene-d10	11.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	17-Octadecen-14-yn-1-ol	264	C18H32O	018202-28-3	43
2	Cyclohexene, 2,4-dimethyl-1-(1-m...	150	C11H18	056763-60-1	38
3	Cyclohexanemethanol, 4-methylene-	126	C8H14O	001004-24-6	37
4	(4-Methyl-cyclohex-3-enyl)-methanol	126	C8H14O	089690-46-0	35
5	.beta.-Pinene	136	C10H16	000127-91-3	27





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ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-13

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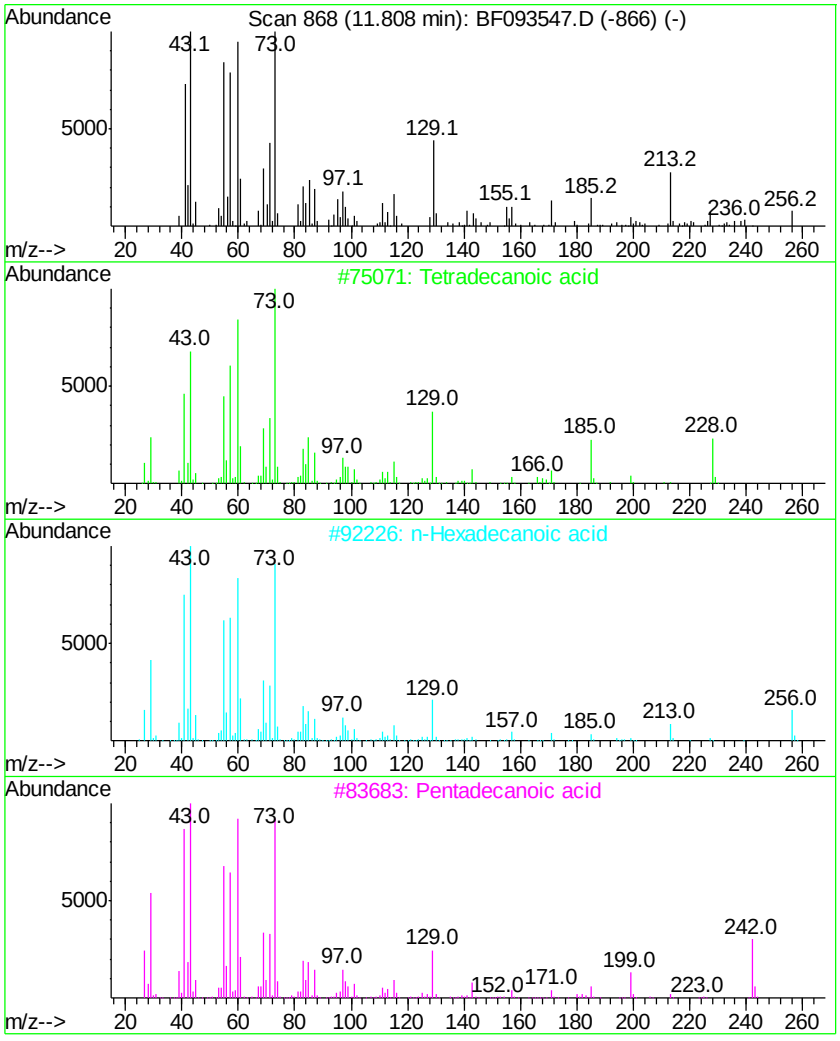
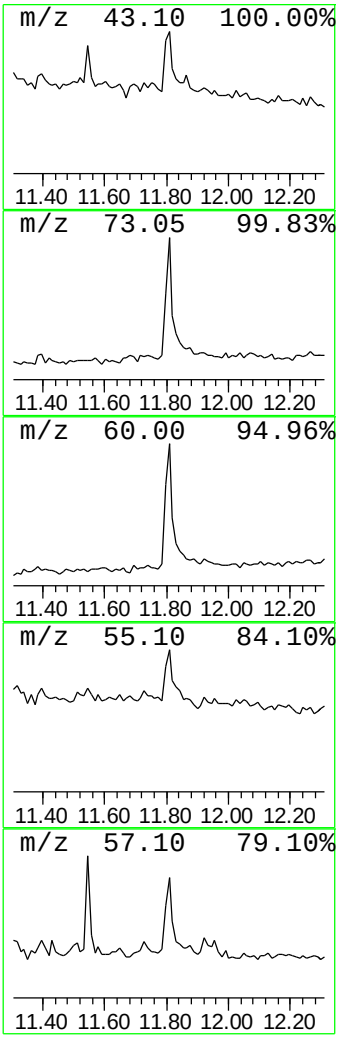
Peak Number 14 Tetradecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.81	3.16 ng	251351	Phenanthrene-d10	11.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	80
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	72
4	Tridecanoic acid	214	C13H26O2	000638-53-9	62
5	n-Decanoic acid	172	C10H20O2	000334-48-5	62





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
2-Pentanone, 4-hy...	4.89	4.9	ng	286519	1	6.74	1178360	20.0
unknown6.52	6.52	67.9	ng	4001930	1	6.74	1178360	20.0
unknown7.97	7.97	3.1	ng	296265	2	8.02	1903690	20.0
Naphthalene, 1,2,...	8.26	2.1	ng	202689	2	8.02	1903690	20.0
Benzocycloheptene	8.40	2.5	ng	238609	2	8.02	1903690	20.0
unknown8.50	8.50	2.4	ng	223798	2	8.02	1903690	20.0
Cyclopentane, 1,2...	8.92	2.1	ng	200235	3	9.77	1939080	20.0
unknown9.02	9.02	2.7	ng	261830	3	9.77	1939080	20.0
Cyclohexanol, 3,3...	9.40	6.4	ng	623655	3	9.77	1939080	20.0
unknown10.16	10.16	2.2	ng	216446	3	9.77	1939080	20.0
Benzenesulfonic a...	10.70	3.9	ng	310065	4	11.26	1589600	20.0
unknown11.13	11.13	4.5	ng	360125	4	11.26	1589600	20.0
Tetradecanoic acid	11.81	3.2	ng	251351	4	11.26	1589600	20.0