LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF081217\
Data File : BF097647.D
Acq On : 12 Aug 2017 22:01
Operator : SJ/JU
Sample : I4631-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VE-4-11

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-BF081117.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	4.746	516	520	532	rBV	50998	128748	4.40%	0.669%
2	5.434	633	637	664	rBV	601378	1402199	47.90%	7.291%
3	7.087	913	918	927	rBV	341388	750917	25.65%	3.905%
4	7.169	927	932	946	rVB	1334479	2291230	78.27%	11.914%
5	7.504	984	989	1002	rBV	473922	676681	23.12%	3.519%
6	7.739	1024	1029	1050	rBV	1519617	2064030	70.51%	10.732%
7	8.416	1139	1144	1160	rBV	1161576	1719177	58.73%	8.939%
8	9.528	1329	1333	1346	rBV	681648	940069	32.11%	4.888%
9	10.286	1458	1462	1467	rBV7	16727	29688	1.01%	0.154%
10	10.392	1476	1480	1484	rVV7	16273	31658	1.08%	0.165%
11	10.445	1484	1489	1497	rVB8	28903	64598	2.21%	0.336%
12	11.122	1601	1604	1606	rBV3	29679	29329	1.00%	0.153%
13	11.310	1630	1636	1646	rVV	2121370	2927232	100.00%	15.221%
14	11.398	1647	1651	1655	rVV4	57262	87387	2.99%	0.454%
15	11.451	1657	1660	1668	rVB7	37582	59768	2.04%	0.311%
16	11.522	1668	1672	1675	rBV5	31199	47881	1.64%	0.249%
17	11.880	1729	1733	1735	rBV	127876	159391	5.45%	0.829%
18	11.904	1735	1737	1742	rVB	116951	148321	5.07%	0.771%
19	11.998	1749	1753	1758	rVB	212764	262926	8.98%	1.367%
20	12.133	1773	1776	1784	rBV9	47613	90799	3.10%	0.472%
21	12.210	1784	1789	1794	rBV3	134062	209613	7.16%	1.090%
22	12.263	1795	1798	1804	rVV	58588	86835	2.97%	0.452%
23	12.351	1809	1813	1823	rVB2	614988	885256	30.24%	4.603%
24	13.010	1923	1925	1929	rVB3	47808	49054	1.68%	0.255%
25	13.657	2030	2035	2043	rBV	866919	1295187	44.25%	6.735%
26	14.757	2217	2222	2227	rBV	499643	674427	23.04%	3.507%
27	17.115	2618	2623	2629	rVB	975852	1228795	41.98%	6.389%
28	18.462	2848	2852	2856	rVB	381407	461365	15.76%	2.399%
29	20.133	3132	3136	3143	rVB	356635	429466	14.67%	2.233%

Sum of corrected areas: 19232027

LSC Report - Integrated Chromatogram

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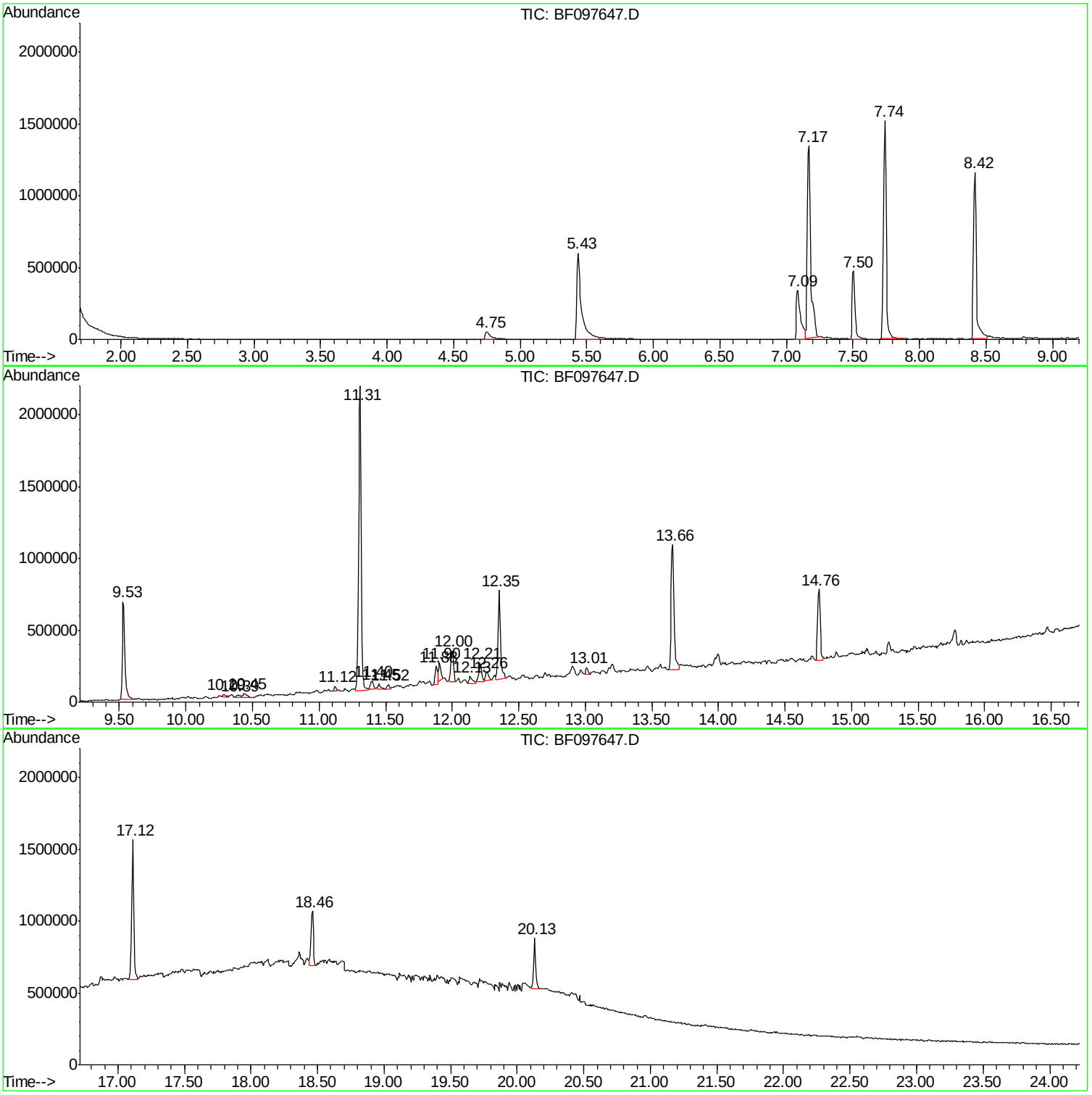
Instrument : BNA_F
ClientSampleId : VE-4-11

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081117.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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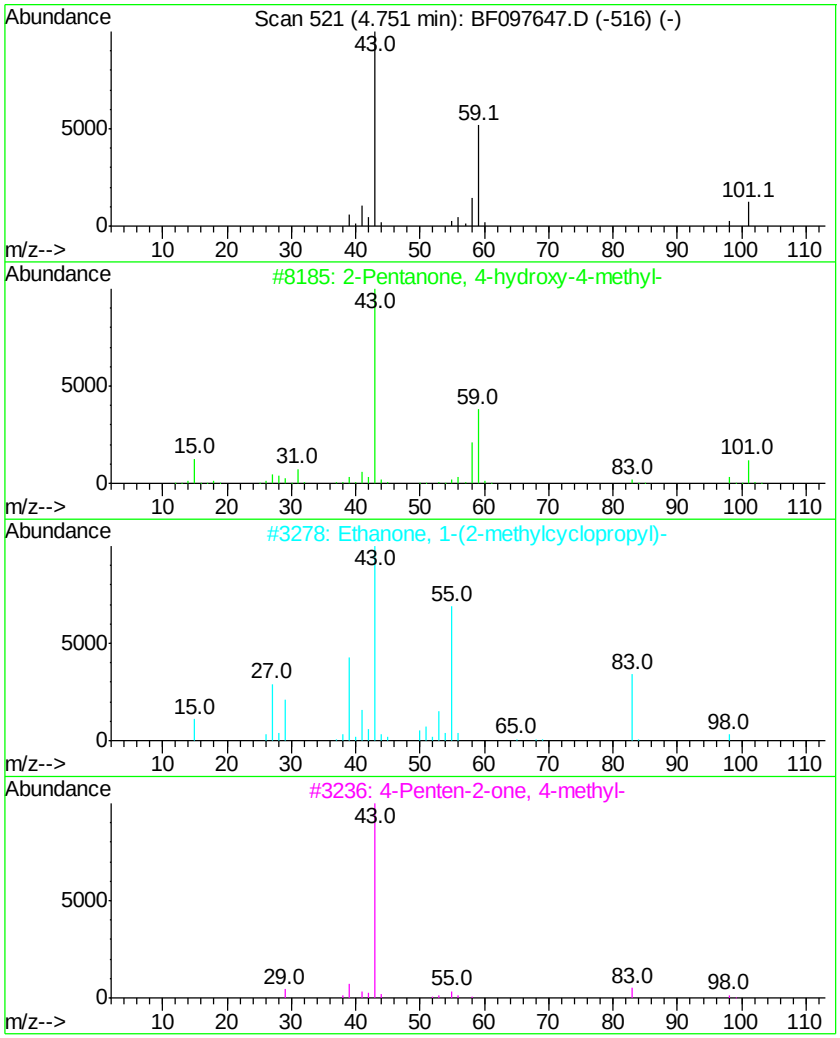
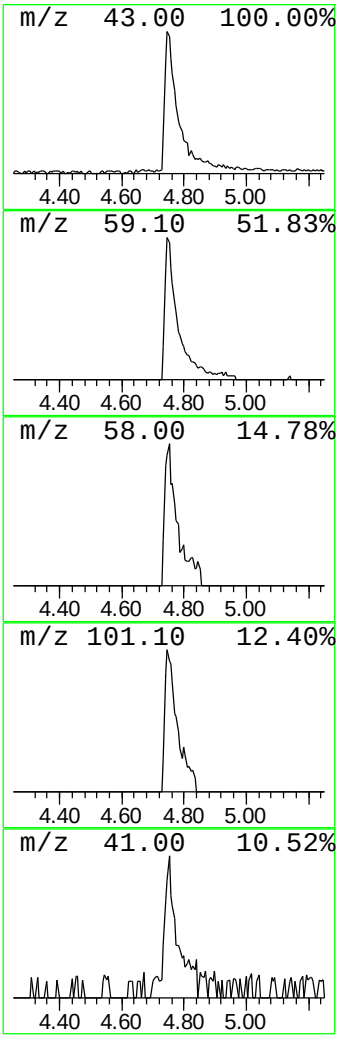
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.75	3.81 ng	128748	1,4-Dichlorobenzene-d4	7.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Ethanone, 1-(2-methylcyclopropyl)-	98	C6H10O	000930-56-3	9
3	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9
4	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9
5	2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	9





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Instrument : BNA_F
ClientSampleId : VE-4-11

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081117.M
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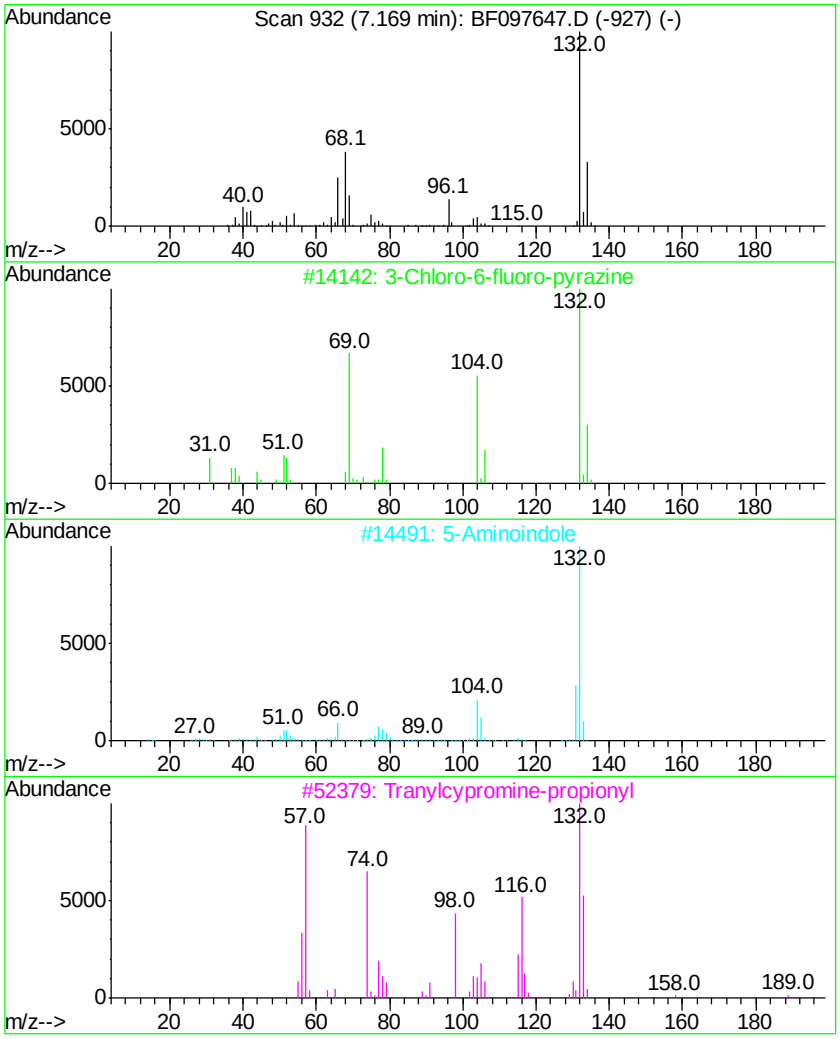
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

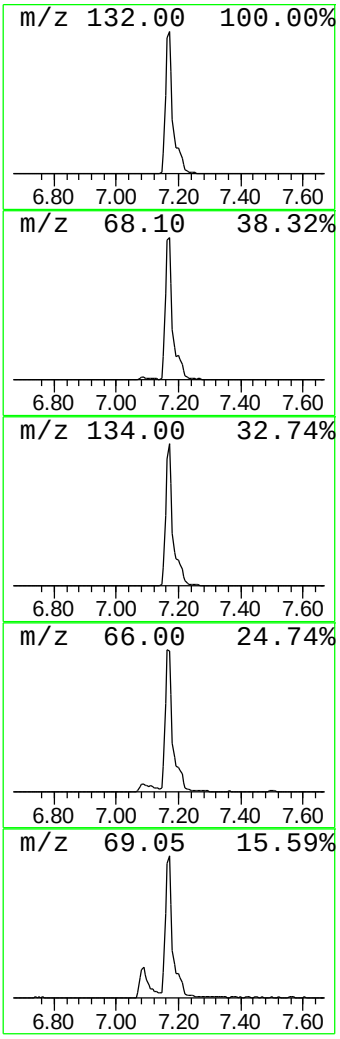
****

Peak Number 2 unknown7.17 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.17	67.72 ng	2291230	1,4-Dichlorobenzene-d4	7.50

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	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





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Instrument : BNA_F
ClientSampleId : VE-4-11

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081117.M
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TIC Library : C:\DATABASE\NIST11.L
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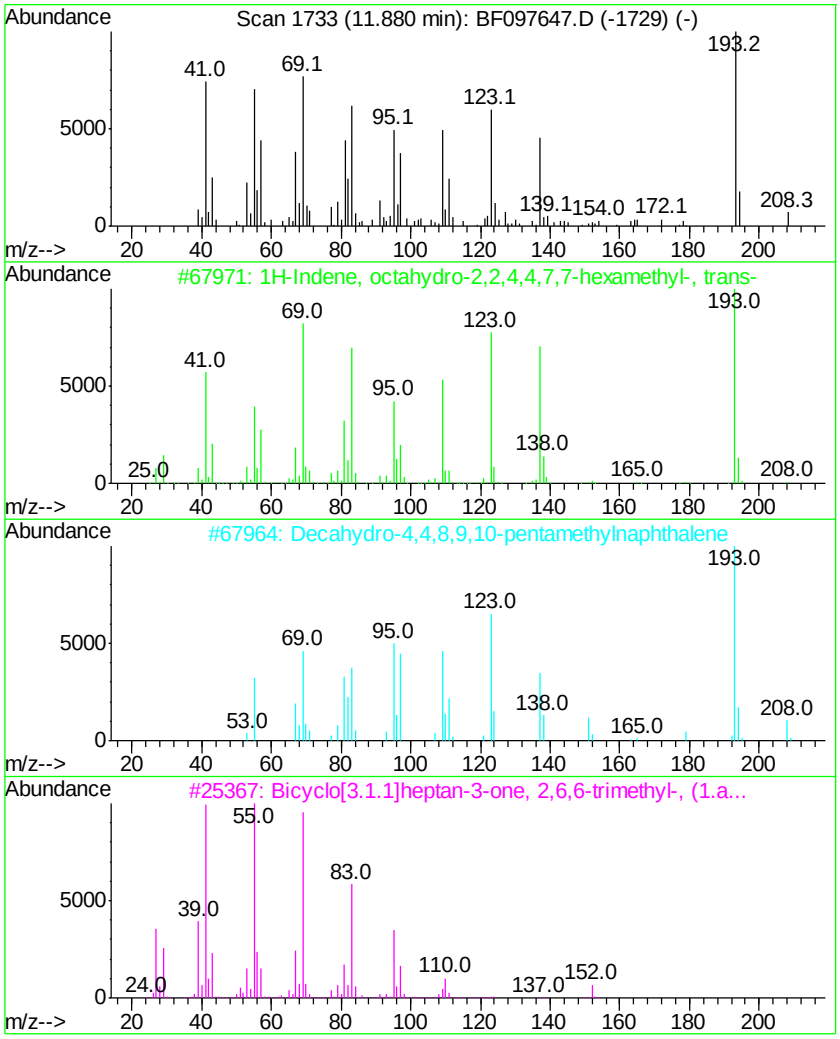
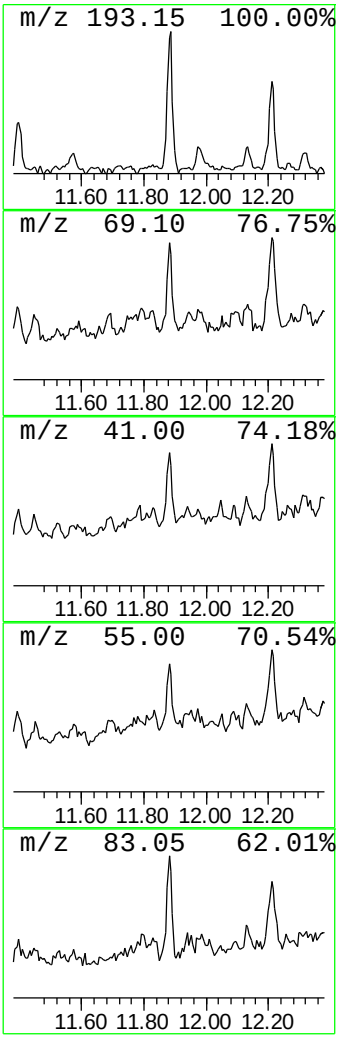
Peak Number 4 1H-Indene, octahydro-2,2,4,... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.88	3.60 ng	159391	Acenaphthene-d10	12.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, octahydro-2,2,4,4,7,7...	208	C15H28	054832-83-6	64
2	Decahydro-4,4,8,9,10-pentamethyl...	208	C15H28	080655-44-3	35
3	Bicyclo[3.1.1]heptan-3-one, 2,6,...	152	C10H16O	015358-88-0	35
4	1-(2-Furyl)-4,4,4-trifluoro-1,3-...	206	C8H5F3O3	000326-90-9	27
5	6-Octenal, 3,7-dimethyl-, (R)-	154	C10H18O	002385-77-5	22





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Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VE-4-11

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081117.M
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TIC Library : C:\DATABASE\NIST11.L
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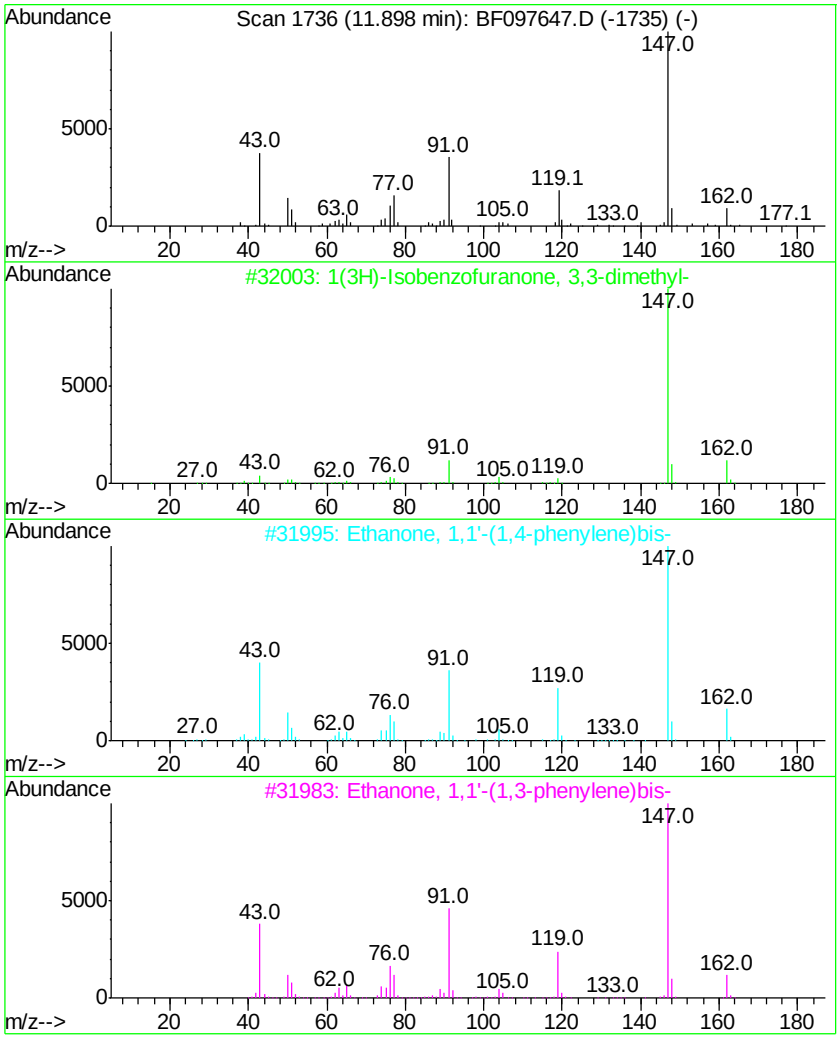
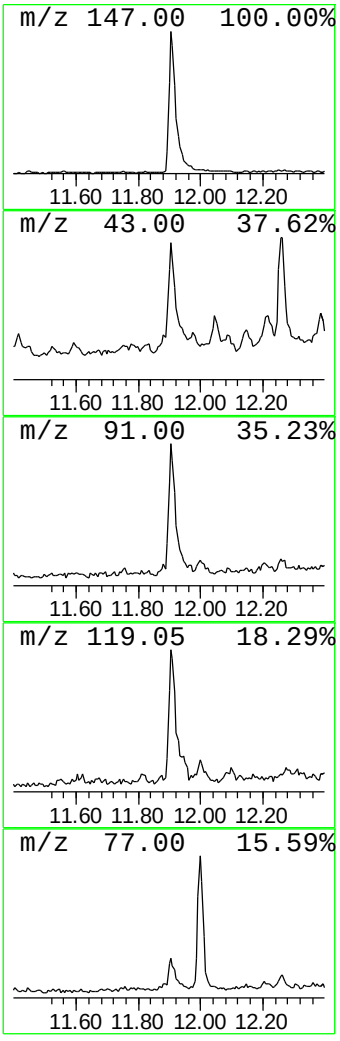
Peak Number 5 1(3H)-Isobenzofuranone, 3,3... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.90	3.35 ng	148321	Acenaphthene-d10	12.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1(3H)-Isobenzofuranone, 3,3-dime...	162	C10H10O2	001689-09-4	86
2	Ethanone, 1,1'-(1,4-phenylene)bis-	162	C10H10O2	001009-61-6	64
3	Ethanone, 1,1'-(1,3-phenylene)bis-	162	C10H10O2	006781-42-6	64
4	2H-Benzotriazole, 2-ethyl-	147	C8H9N3	016584-04-6	59
5	Pyrido[2,3-d]pyrimidin-4(1H)-one	147	C7H5N3O	024410-19-3	59





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Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VE-4-11

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081117.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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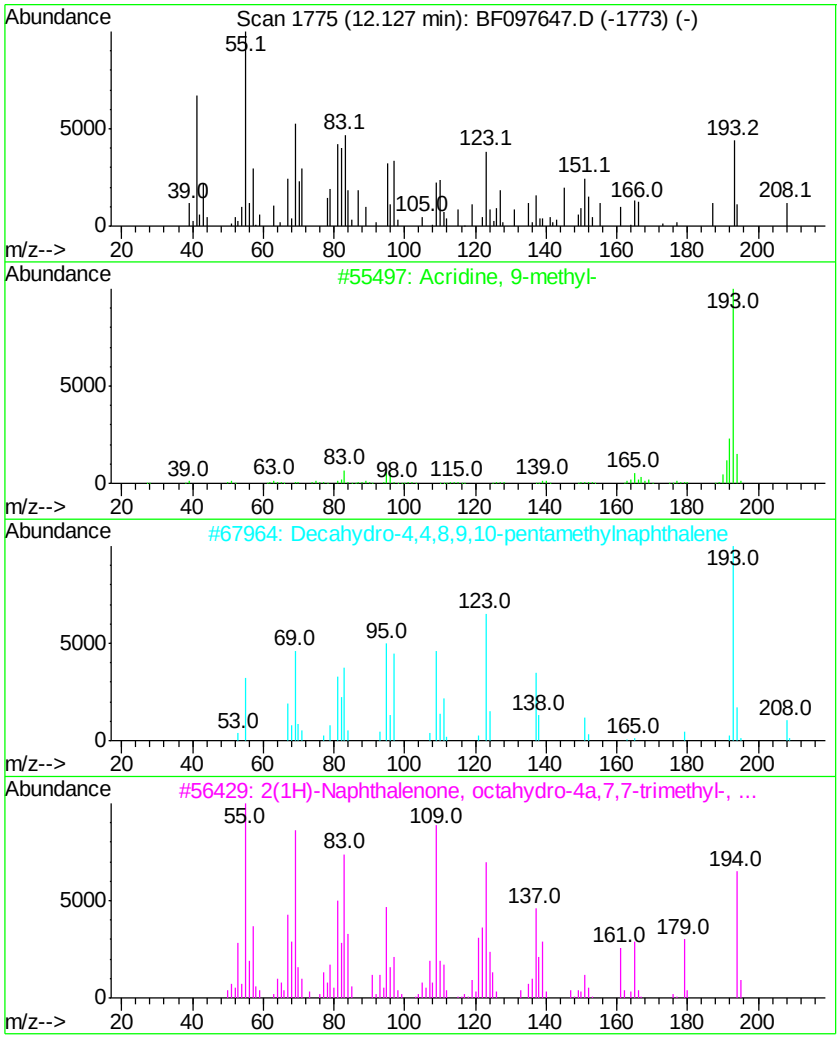
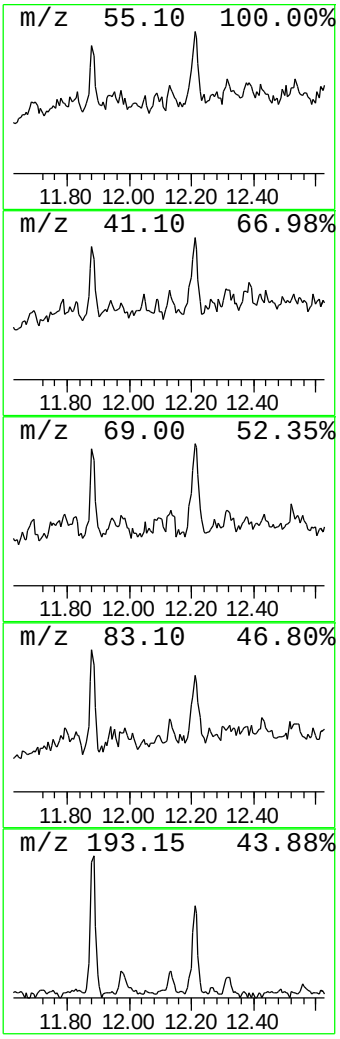
Peak Number 6 Acridine, 9-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.13	2.05 ng	90799	Acenaphthene-d10	12.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acridine, 9-methyl-	193	C14H11N	000611-64-3	84
2	Decahydro-4,4,8,9,10-pentamethyl...	208	C15H28	080655-44-3	70
3	2(1H)-Naphthalenone, octahydro-4...	194	C13H22O	054699-31-9	40
4	8-Oxabicyclo[3.2.1]oct-6-en-3-on...	152	C9H12O2	049747-05-9	38
5	Borinic acid, diethyl-, 3,3,5-tr...	208	C13H25BO	057387-76-5	30





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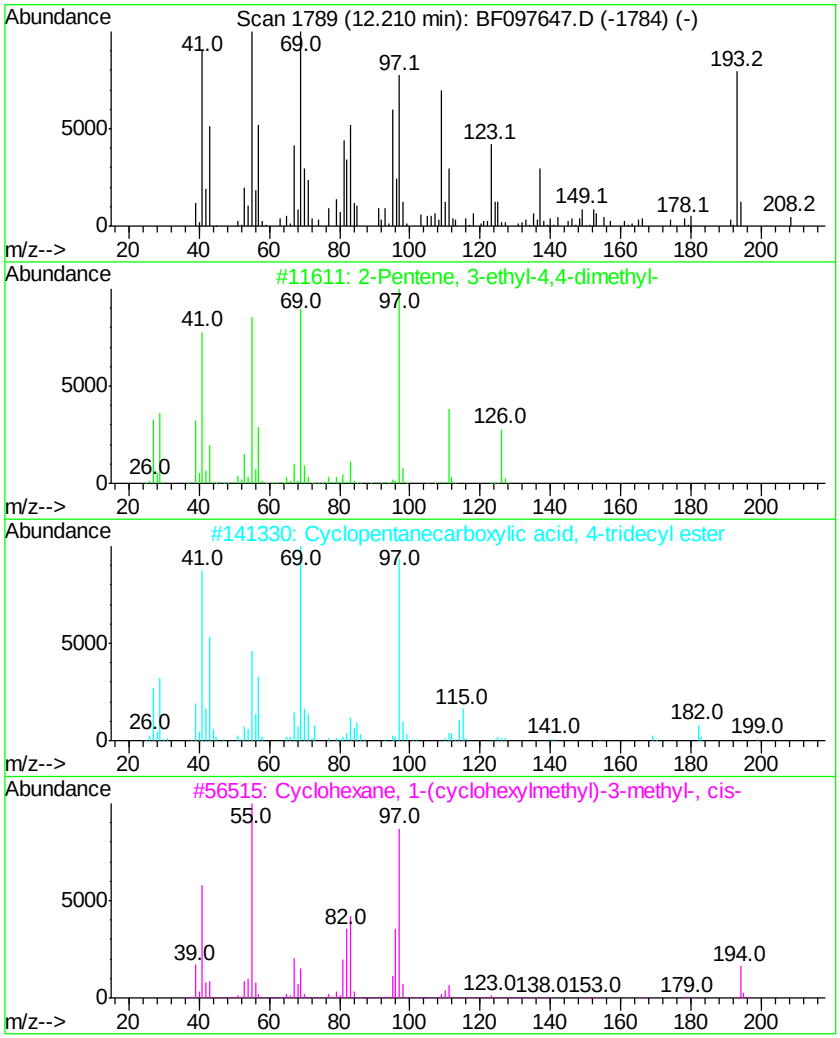
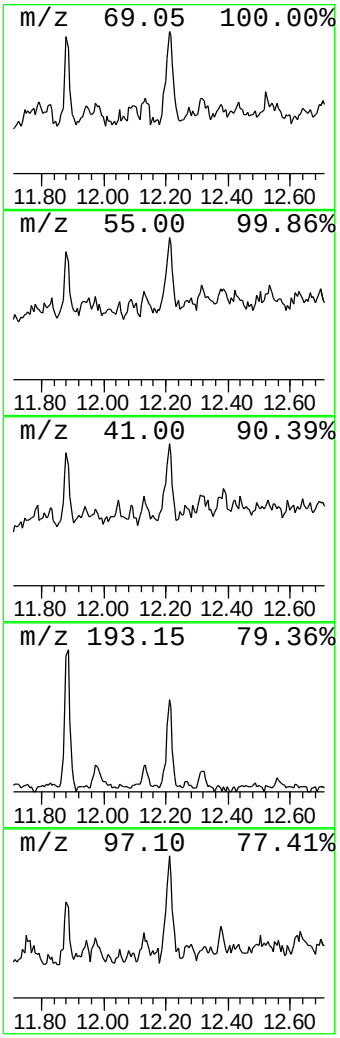
Peak Number 7 unknown12.21 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.21	4.74 ng	209613	Acenaphthene-d10	12.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentene, 3-ethyl-4,4-dimethyl-	126	C9H18	053907-59-8	27
2	Cyclopentanecarboxylic acid, 4-t...	296	C19H36O2	1000280-58-6	22
3	Cyclohexane, 1-(cyclohexylmethyl...	194	C14H26	054823-96-0	18
4	(5-Ethylcyclopent-1-enyl)methanol	126	C8H14O	036431-59-1	14
5	Cyclopentane, (1-methylbutyl)-	140	C10H20	004737-43-3	11





Tentatively Identified Compound (LSC) summary

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.75	3.8	ng	128748	1	7.50	676681	20.0
unknown7.17	7.17	67.7	ng	2291230	1	7.50	676681	20.0
1H-Indene, octahy...	11.88	3.6	ng	159391	3	12.35	885256	20.0
1(3H)-Isobenzofur...	11.90	3.4	ng	148321	3	12.35	885256	20.0
Acridine, 9-methyl-	12.13	2.0	ng	90799	3	12.35	885256	20.0
unknown12.21	12.21	4.7	ng	209613	3	12.35	885256	20.0