LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF043017\
Data File : BF094716.D
Acq On : 30 Apr 2017 15:59
Operator : SJ/MA
Sample : I2860-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HW-1

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-BF041717.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	3.390	244	247	263	rBV	464815	488991	15.16%	2.268%
2	3.931	334	339	342	rBV	1195144	1356347	42.06%	6.291%
3	4.331	404	407	420	rBV	466726	516899	16.03%	2.398%
4	4.707	467	471	479	rVB	248295	251985	7.81%	1.169%
5	5.390	584	587	601	rBV	286115	330869	10.26%	1.535%
6	5.519	605	609	617	rBV	1204259	1098915	34.08%	5.097%
7	5.766	647	651	657	rBV	752106	661200	20.50%	3.067%
8	5.943	677	681	685	rBV	2150929	1985399	61.56%	9.209%
9	6.419	756	762	765	rBV	1532329	1624101	50.36%	7.533%
10	7.254	900	904	913	rBV	935166	913529	28.33%	4.237%
11	8.578	1125	1129	1133	rBV	3183054	3224913	100.00%	14.959%
12	9.084	1211	1215	1222	rVB	210379	198181	6.15%	0.919%
13	9.389	1263	1267	1273	rBV2	1091829	1045887	32.43%	4.851%
14	10.366	1429	1433	1445	rBV	871866	883944	27.41%	4.100%
15	11.213	1573	1577	1587	rBV	1062478	1051225	32.60%	4.876%
16	11.948	1698	1702	1712	rBV2	149239	184896	5.73%	0.858%
17	12.924	1863	1868	1873	rBV	368868	427471	13.26%	1.983%
18	13.195	1908	1914	1917	rBV	2446321	2776095	86.08%	12.877%
19	14.360	2109	2112	2120	rVB8	23318	44575	1.38%	0.207%
20	14.466	2125	2130	2136	rBV	889606	907227	28.13%	4.208%
21	14.513	2136	2138	2143	rVB	58285	57202	1.77%	0.265%
22	15.318	2271	2275	2279	rBV2	30020	35683	1.11%	0.166%
23	15.483	2299	2303	2313	rBV	776185	821690	25.48%	3.811%
24	15.571	2314	2318	2323	rVB	39276	42339	1.31%	0.196%
25	16.095	2402	2407	2416	rBV	549876	629059	19.51%	2.918%

Sum of corrected areas: 21558622

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Instrument : BNA_F
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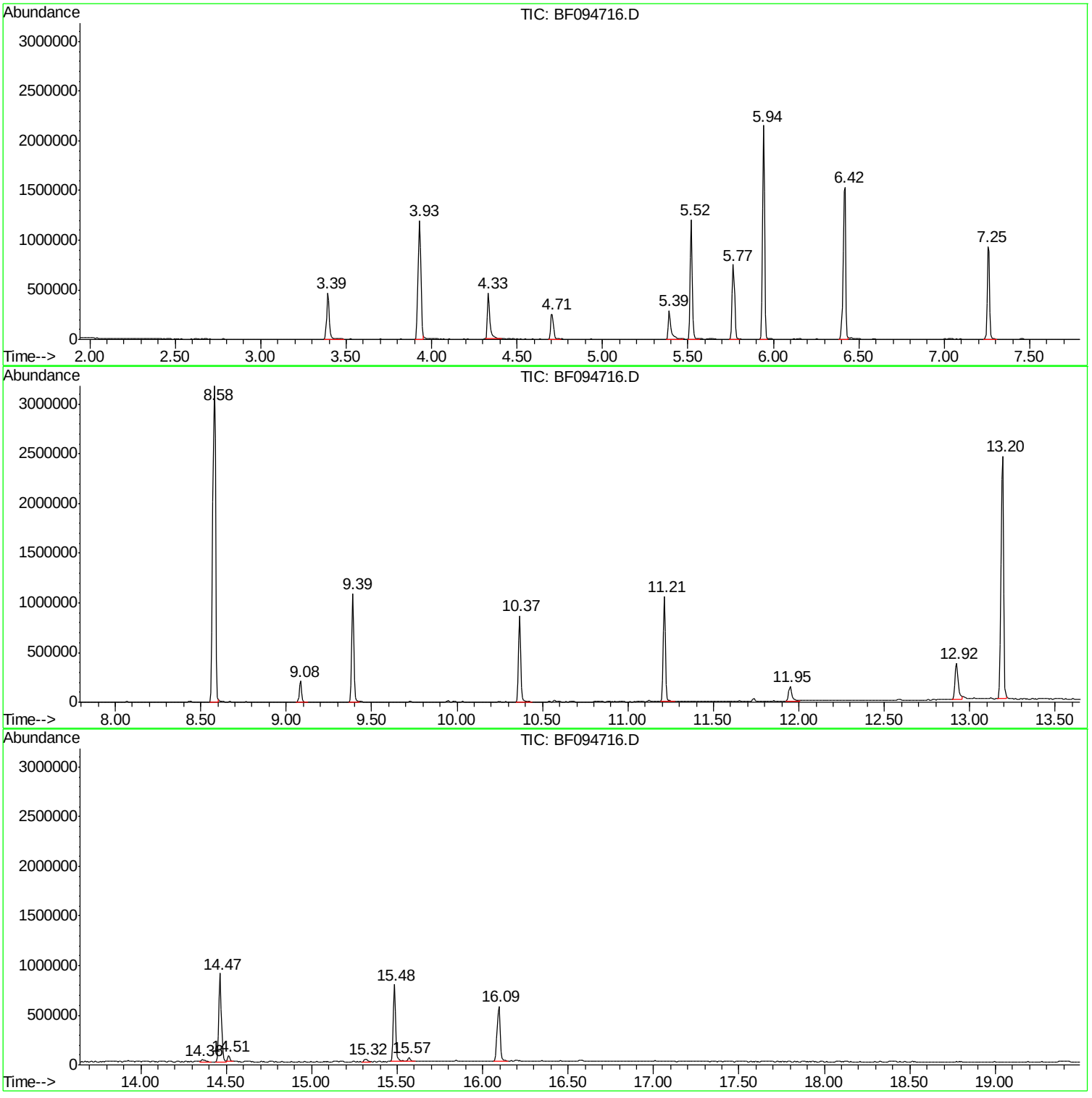
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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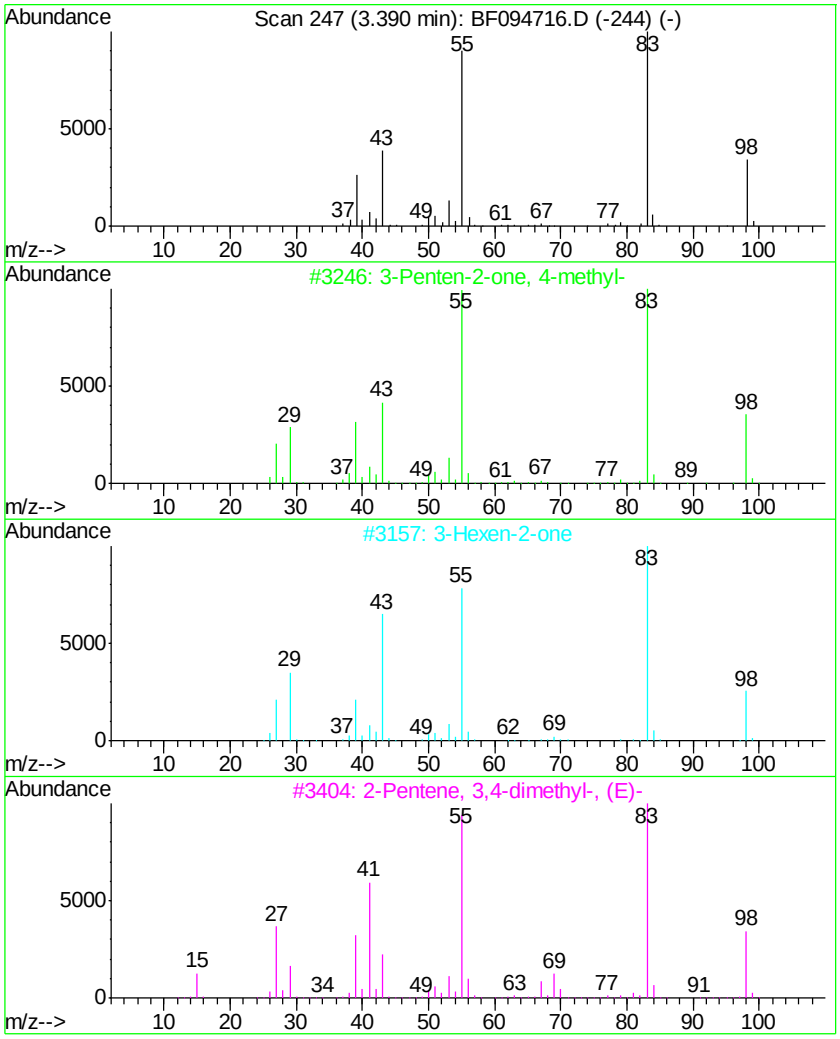
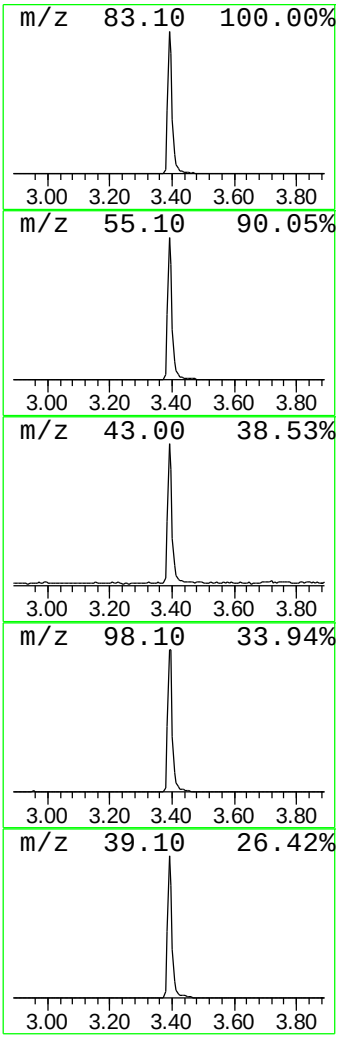
****

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.39	14.79 ng	488991	1,4-Dichlorobenzene-d4	5.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	95
2	3-Hexen-2-one	98	C6H10O	000763-93-9	91
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4	2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	86
5	2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	86





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Instrument : BNA_F
ClientSampleId : HW-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.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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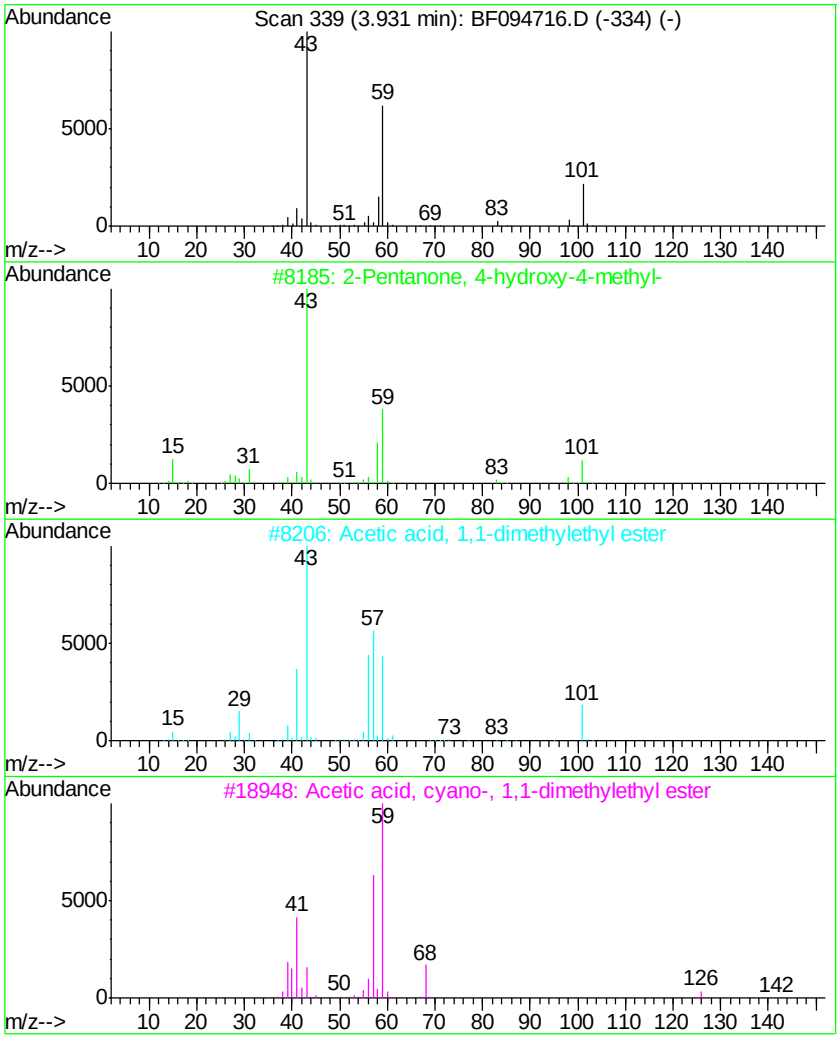
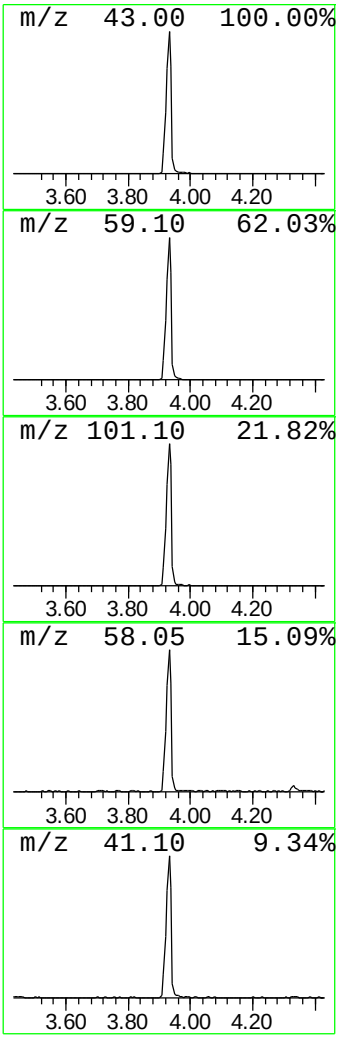
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.93	41.03 ng	1356350	1,4-Dichlorobenzene-d4	5.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





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Operator : SJ/MA
Sample : I2860-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HW-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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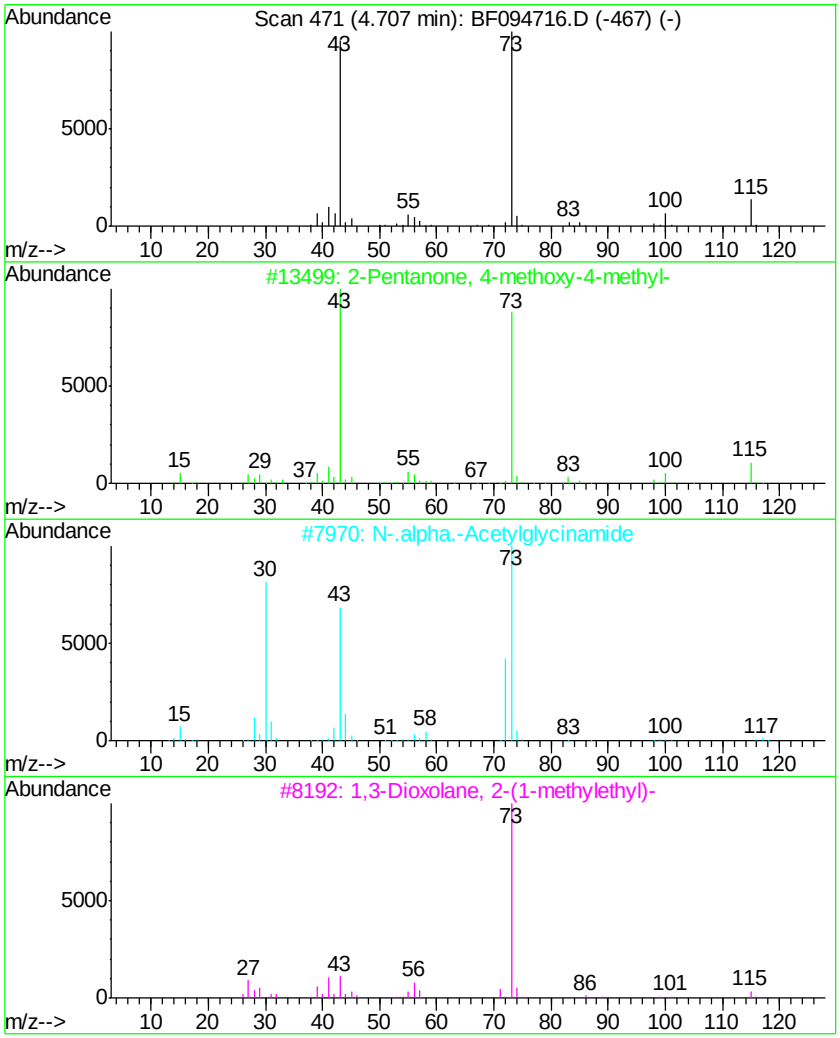
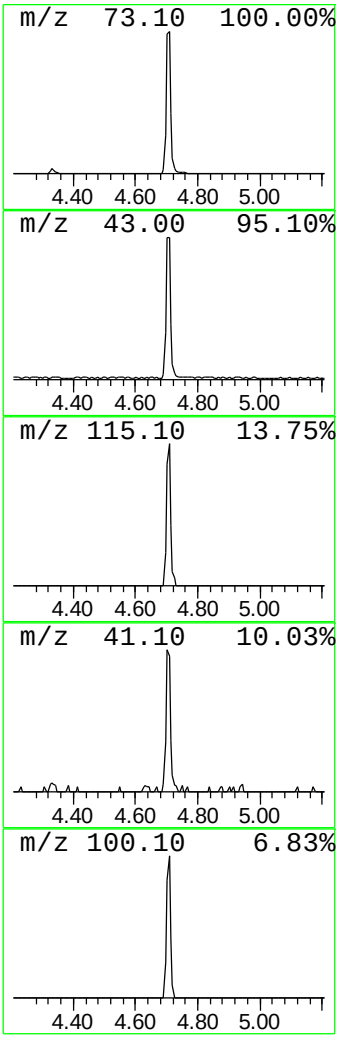
Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.71	7.62 ng	251985	1,4-Dichlorobenzene-d4	5.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2	N-.alpha.-Acetylglycinamide	116	C4H8N2O2	002620-63-5	33
3	1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	17
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	9





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Instrument : BNA_F
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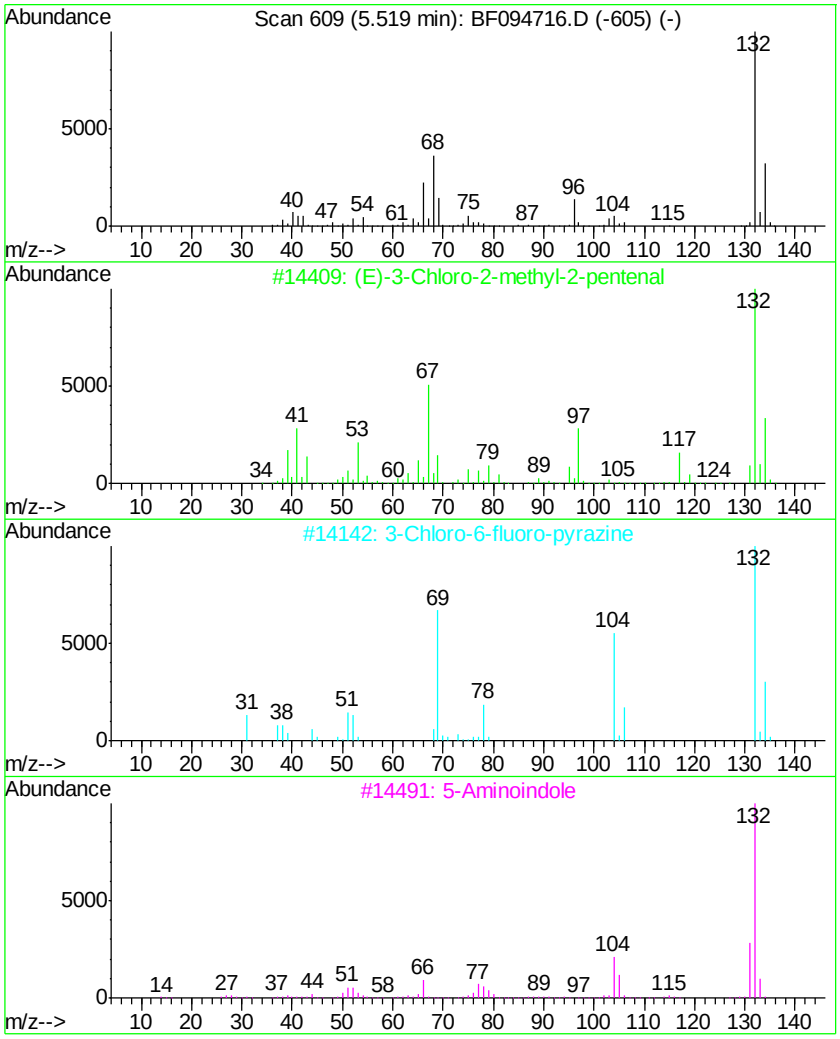
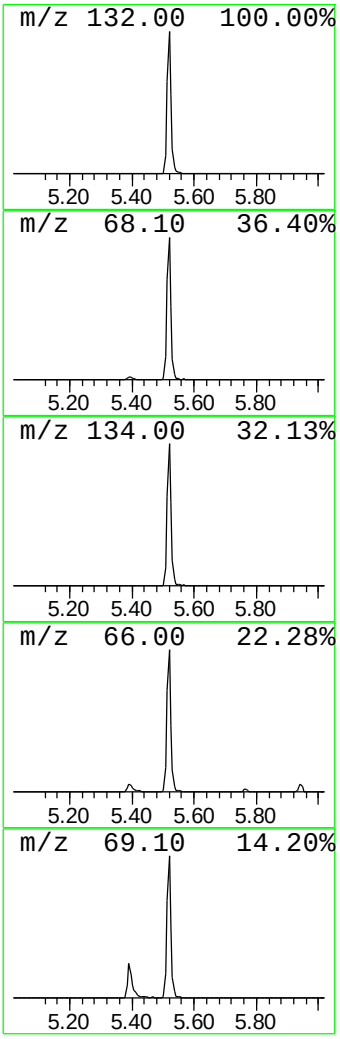
Peak Number 4 unknown5.52 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.52	33.24 ng	1098920	1,4-Dichlorobenzene-d4	5.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
5	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9





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Instrument : BNA_F
ClientSampleId : HW-1

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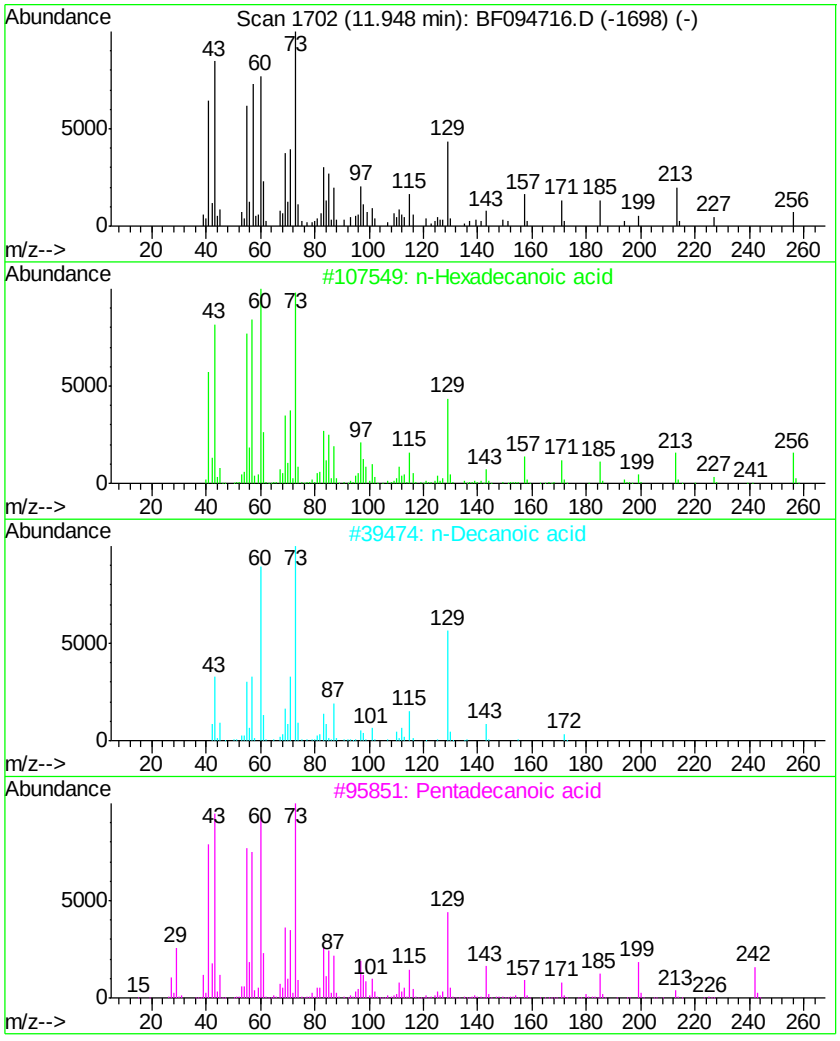
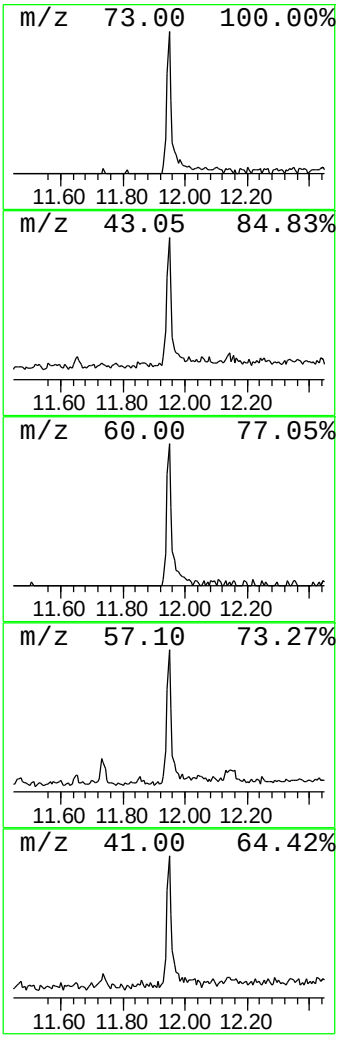
Peak Number 6 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.95	3.52 ng	184896	Phenanthrene-d10	11.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	n-Decanoic acid	172	C10H20O2	000334-48-5	92
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	86
5	Tridecanoic acid	214	C13H26O2	000638-53-9	76





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Sample : I2860-03
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Instrument : BNA_F
ClientSampleId : HW-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.M
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TIC Library : C:\DATABASE\NIST11.L
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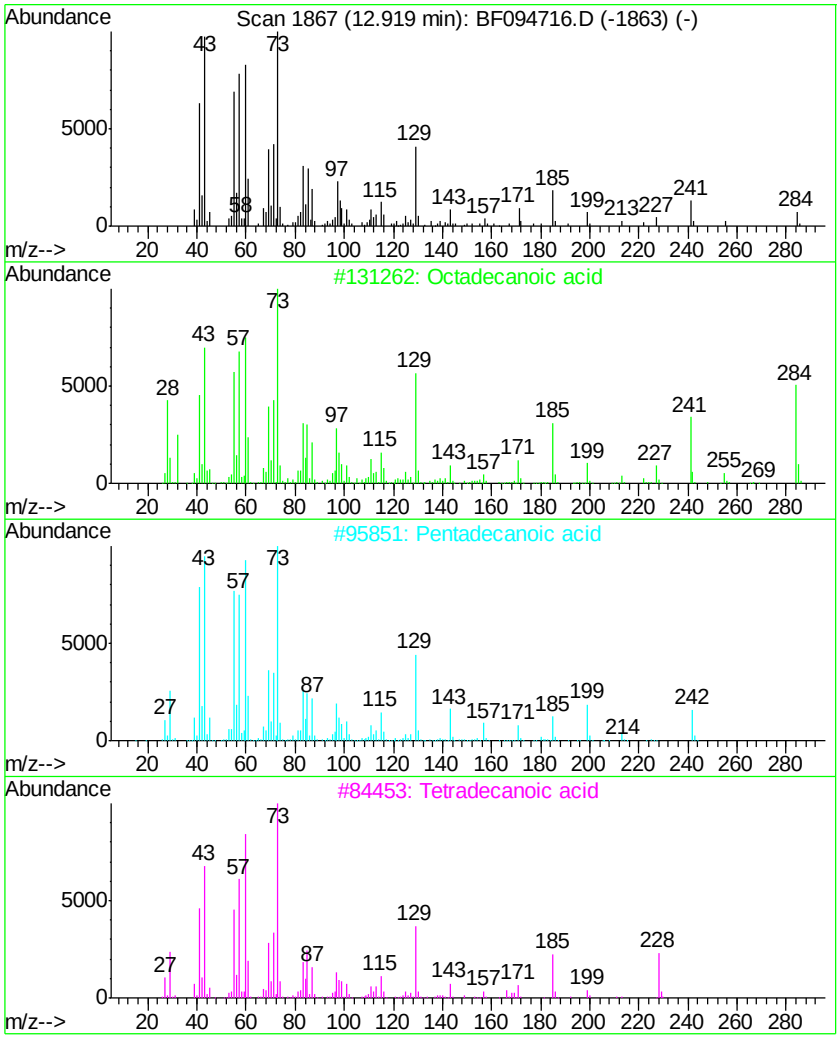
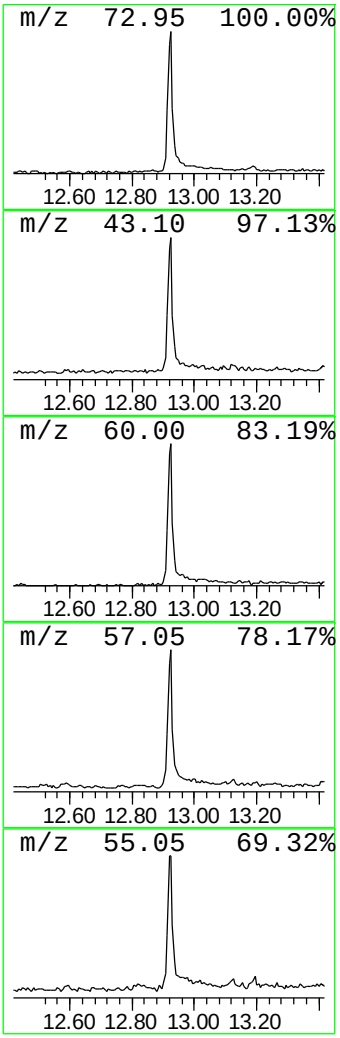
Peak Number 7 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.92	9.42 ng	427471	Chrysene-d12	14.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	94
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
5	n-Decanoic acid	172	C10H20O2	000334-48-5	49





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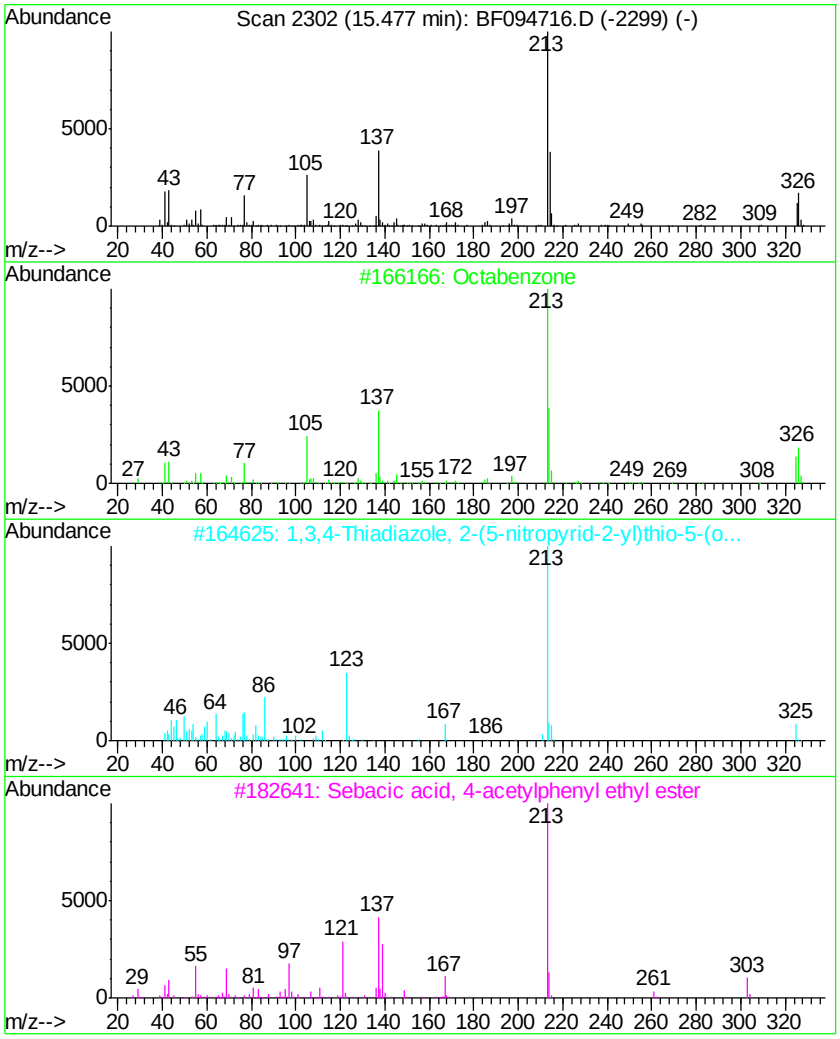
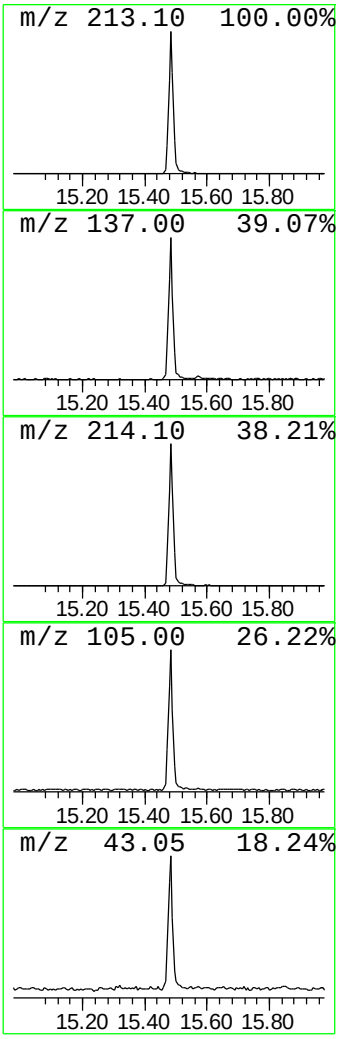
Peak Number 8 Octabenzone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.48	26.12 ng	821690	Perylene-d12	16.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octabenzone	326	C21H26O3	001843-05-6	99
2	1,3,4-Thiadiazole, 2-(5-nitropyr...	325	C10H7N5O4S2	1000260-74-4	37
3	Sebacic acid, 4-acetylphenyl eth...	348	C20H28O5	1000354-96-0	28
4	Pyrimidine, 2,4-diamino-6-ethyl-...	214	C12H14N4	027653-49-2	12
5	Harmaline	214	C13H14N2O	000304-21-2	12





Tentatively Identified Compound (LSC) summary

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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
3-Penten-2-one, 4...	3.39	14.8	ng	488991	1	5.77	661200	20.0
2-Pentanone, 4-hy...	3.93	41.0	ng	1356350	1	5.77	661200	20.0
2-Pentanone, 4-me...	4.71	7.6	ng	251985	1	5.77	661200	20.0
unknown5.52	5.52	33.2	ng	1098920	1	5.77	661200	20.0
n-Hexadecanoic acid	11.95	3.5	ng	184896	4	11.21	1051230	20.0
Octadecanoic acid	12.92	9.4	ng	427471	5	14.47	907227	20.0
Octabenzone	15.48	26.1	ng	821690	6	16.09	629059	20.0