LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100617\
Data File : BF099164.D
Acq On : 6 Oct 2017 23:03
Operator : SJ/JU
Sample : I5516-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-5

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-BF092317.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	2.163	8	13	20	rVB	302312	392614	14.82%	2.272%
2	2.993	149	154	162	rVB	32436	51243	1.93%	0.297%
3	3.610	254	259	270	rBV	150649	225766	8.52%	1.307%
4	4.481	401	407	410	rBV	2131897	2648511	100.00%	15.329%
5	4.534	412	416	421	rVB2	23936	28282	1.07%	0.164%
6	4.734	445	450	454	rBV	45233	46470	1.75%	0.269%
7	5.081	506	509	518	rVB	155321	154049	5.82%	0.892%
8	5.481	574	577	587	rVB	602999	567366	21.42%	3.284%
9	6.487	739	748	756	rBV2	399925	547742	20.68%	3.170%
10	6.628	769	772	776	rBV	1195756	990075	37.38%	5.730%
11	6.863	808	812	815	rBV	808712	652551	24.64%	3.777%
12	7.016	834	838	842	rBV	1347460	1122003	42.36%	6.494%
13	7.422	903	907	910	rBV	1007268	866969	32.73%	5.018%
14	7.504	916	921	925	rBV3	18620	29323	1.11%	0.170%
15	7.581	930	934	936	rBV	102568	97441	3.68%	0.564%
16	8.145	1026	1030	1033	rBV	977493	890296	33.61%	5.153%
17	9.216	1207	1212	1215	rBV	2043848	1677038	63.32%	9.707%
18	9.610	1275	1279	1282	rBV	401972	306802	11.58%	1.776%
19	9.822	1311	1315	1319	rBV	93368	93008	3.51%	0.538%
20	9.898	1323	1328	1332	rBV	962550	829346	31.31%	4.800%
21	10.033	1349	1351	1357	rBV4	19832	30621	1.16%	0.177%
22	10.098	1359	1362	1366	rVB3	44219	47012	1.78%	0.272%
23	10.316	1397	1399	1403	rVB	101613	90744	3.43%	0.525%
24	10.539	1433	1437	1439	rBV	40977	49569	1.87%	0.287%
25	10.686	1458	1462	1468	rVB	721076	686987	25.94%	3.976%
26	10.792	1477	1480	1489	rVB	155507	173376	6.55%	1.003%
27	10.980	1509	1512	1516	rBV4	29476	43556	1.64%	0.252%
28	11.239	1553	1556	1558	rBV	98161	73721	2.78%	0.427%
29	11.269	1558	1561	1567	rVB3	31371	38896	1.47%	0.225%
30	11.386	1577	1581	1584	rBV	1081543	975480	36.83%	5.646%
31	11.910	1666	1670	1678	rBV2	226868	279244	10.54%	1.616%
32	12.692	1800	1803	1810	rBV	106810	122107	4.61%	0.707%
33	12.968	1845	1850	1853	rBV	1594535	1556837	58.78%	9.011%
34	13.374	1916	1919	1922	rBV	49599	44086	1.66%	0.255%

LSC Area Percent Report

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Data File : BF099164.D
Acq On : 6 Oct 2017 23:03
Operator : SJ/JU
Sample : I5516-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-5

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-BF092317.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.021	2025	2029	2038	rVB	713351	630242	23.80%	3.648%
36	14.115	2042	2045	2048	rVB3	33735	27823	1.05%	0.161%
37	15.498	2275	2280	2287	rVB2	112431	163076	6.16%	0.944%
38	15.933	2349	2354	2360	rVB4	16747	27044	1.02%	0.157%

Sum of corrected areas: 17277316

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Operator : SJ/JU
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Instrument : BNA_F
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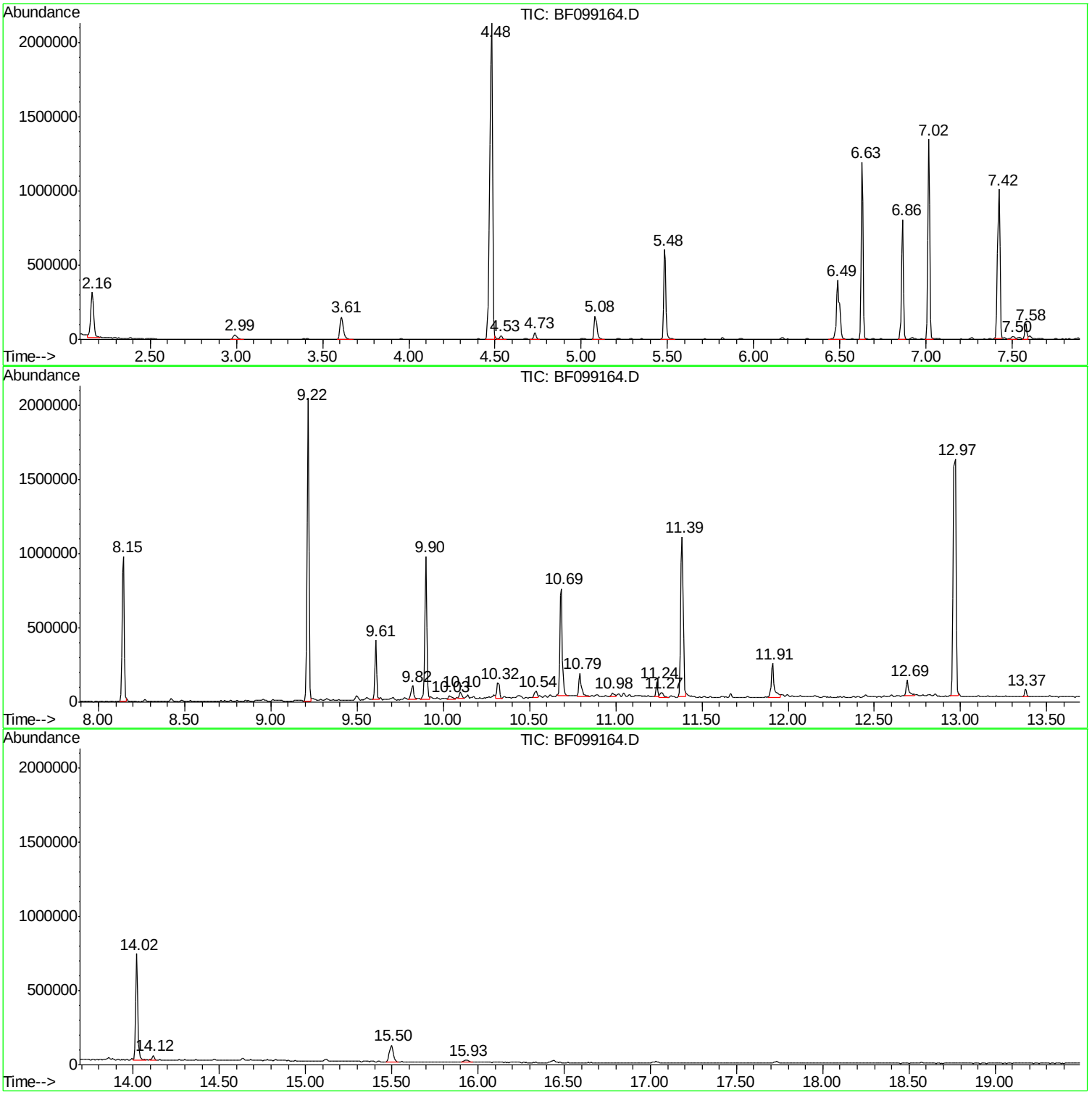
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

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Operator : SJ/JU
Sample : I5516-01
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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

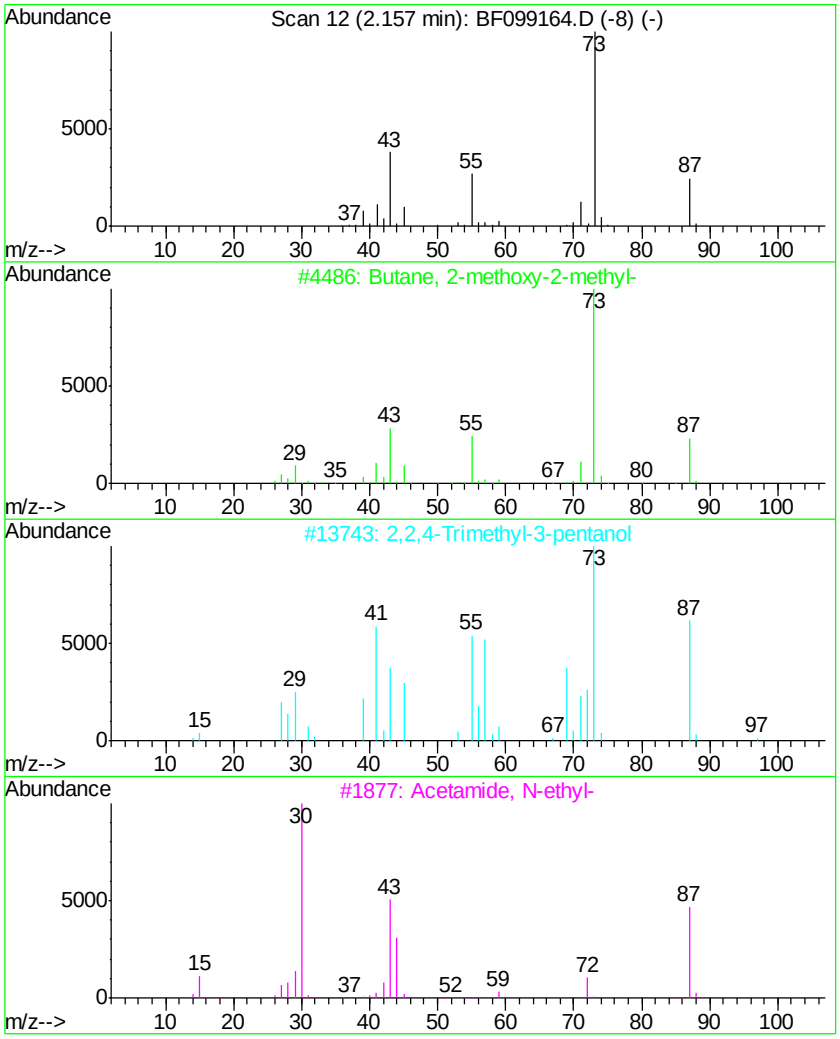
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

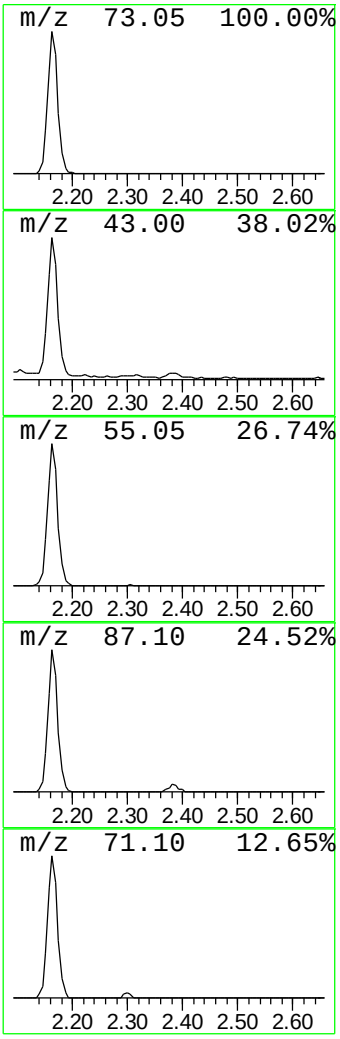
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.16	12.03 ng	392614	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





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Operator : SJ/JU
Sample : I5516-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

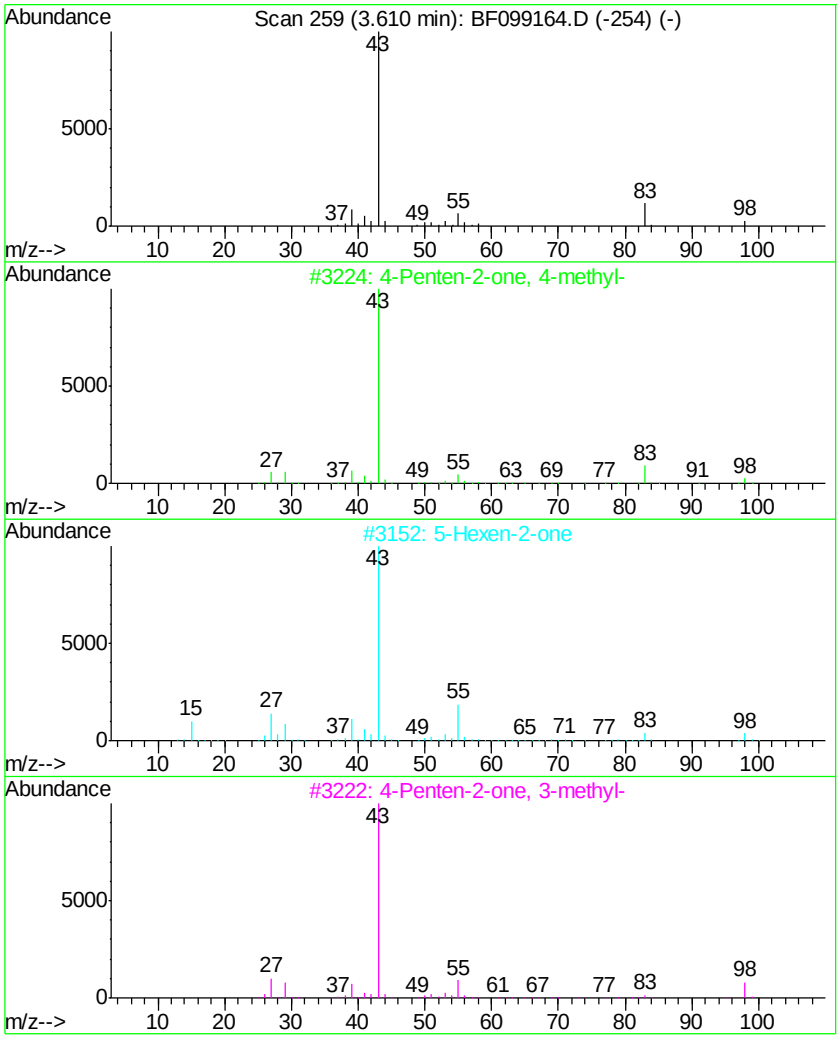
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

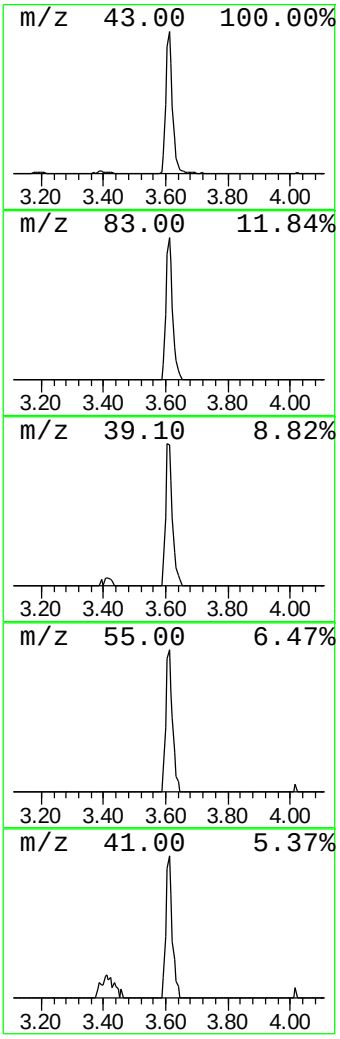
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.61	6.92 ng	225766	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	86
2	5-Hexen-2-one	98	C6H10O	000109-49-9	47
3	4-Penten-2-one, 3-methyl-	98	C6H10O	000758-87-2	37
4	2-Pentanone, 3-methylene-	98	C6H10O	004359-77-7	17
5	Isoxazole, 5-methyl-	83	C4H5NO	005765-44-6	9





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Operator : SJ/JU
Sample : I5516-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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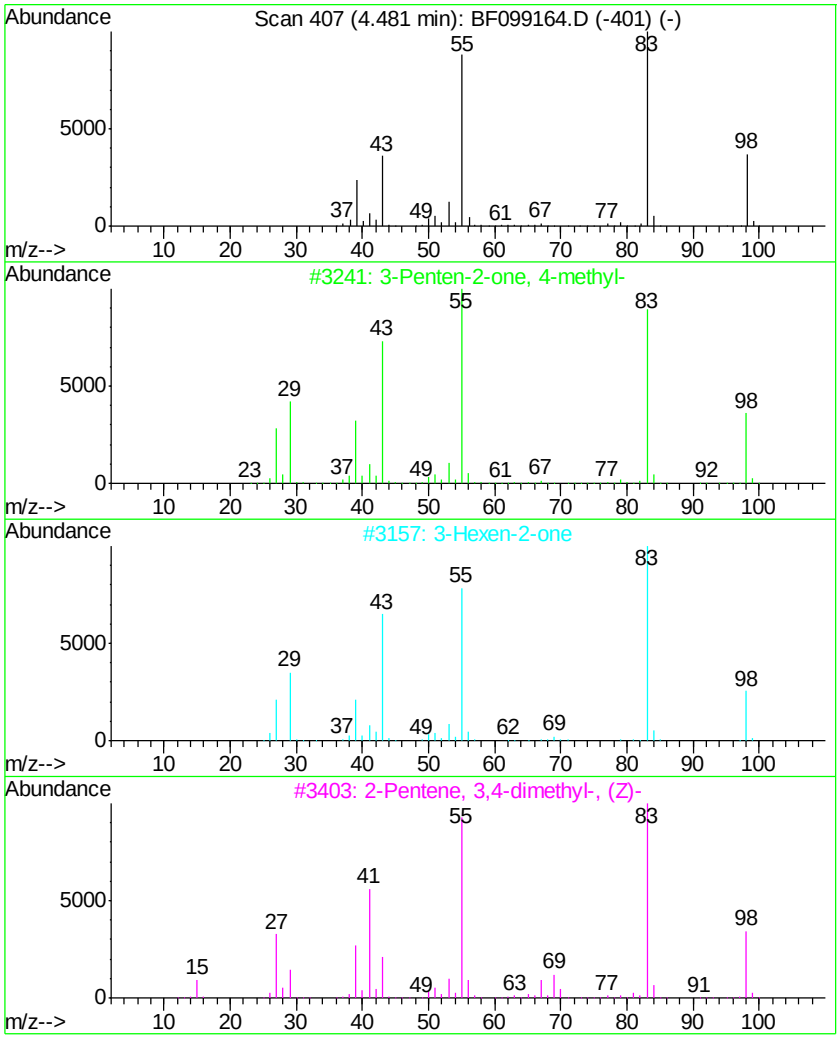
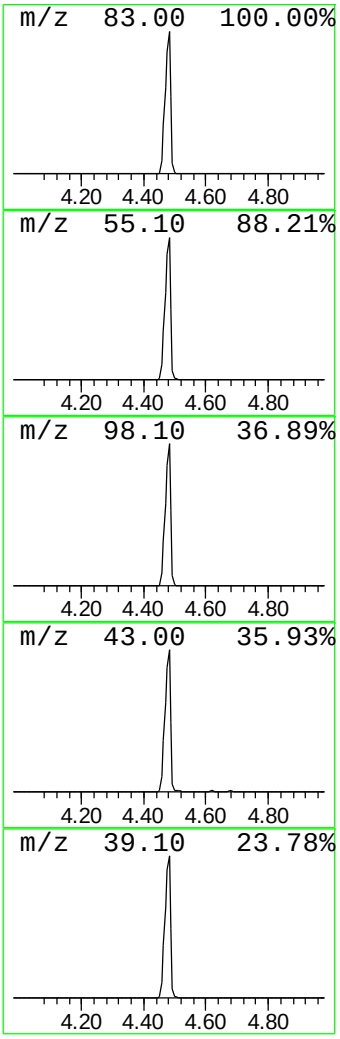
Peak Number 3 3-Penten-2-one, 4-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.48	81.17 ng	2648510	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2	3-Hexen-2-one	98	C6H10O	000763-93-9	91
3	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
4	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
5	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80





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Operator : SJ/JU
Sample : I5516-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

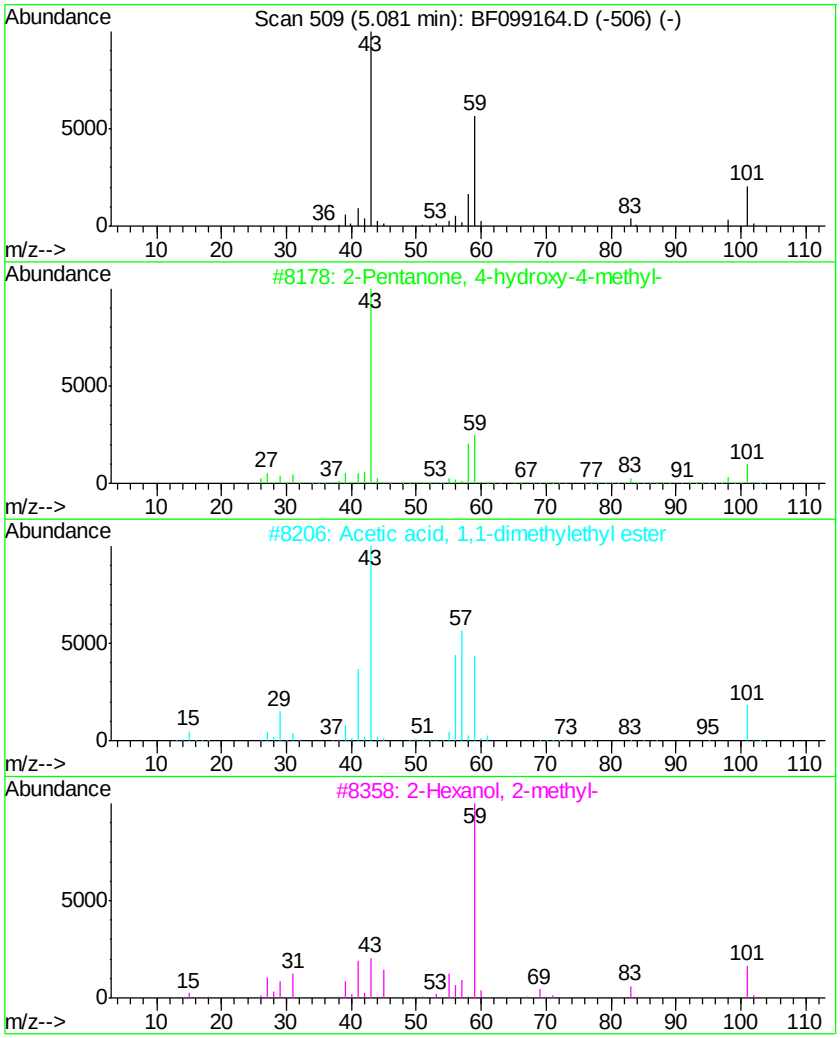
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

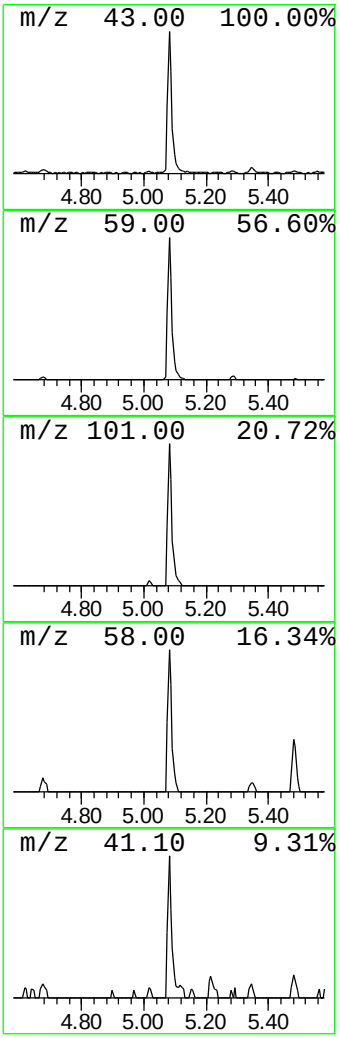
****

Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.08	4.72 ng	154049	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9





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Operator : SJ/JU
Sample : I5516-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

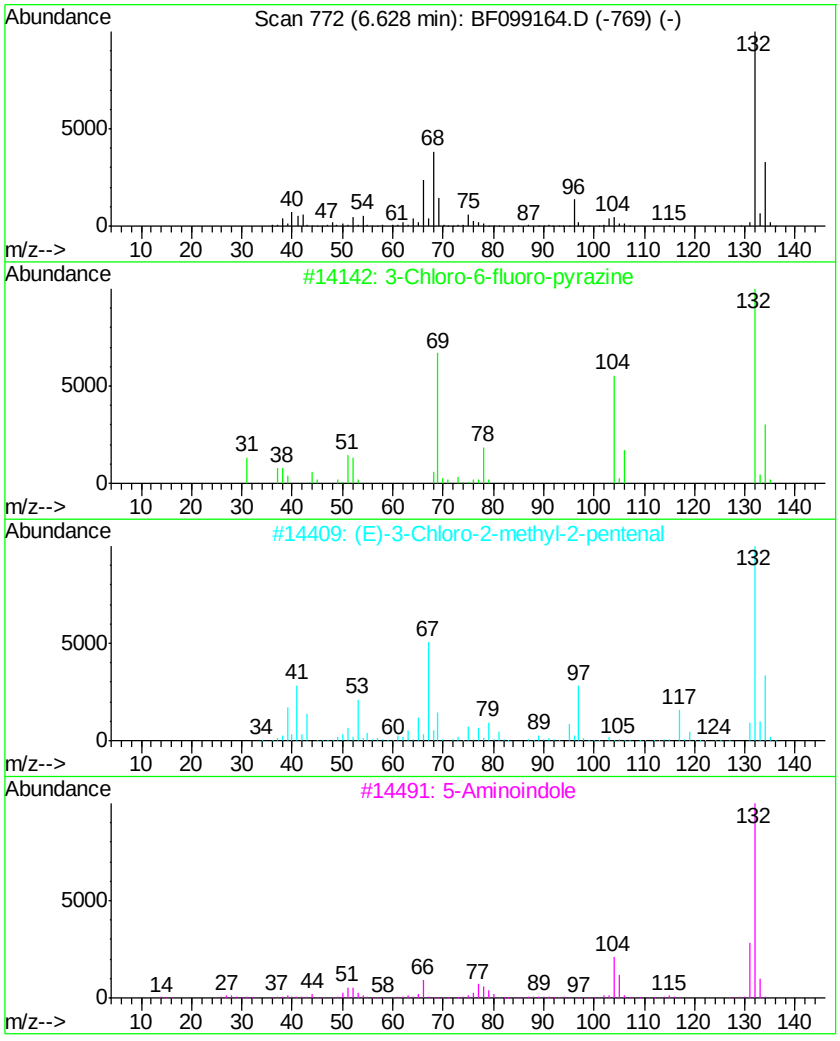
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

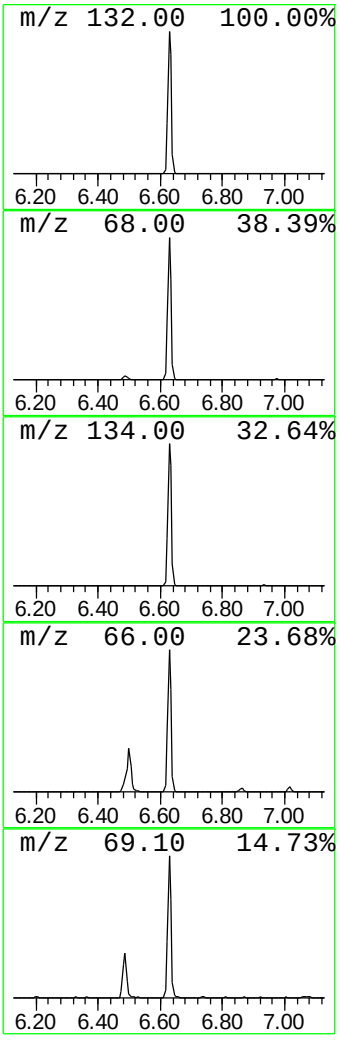
****

Peak Number 5 unknown6.63 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	30.34 ng	990075	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

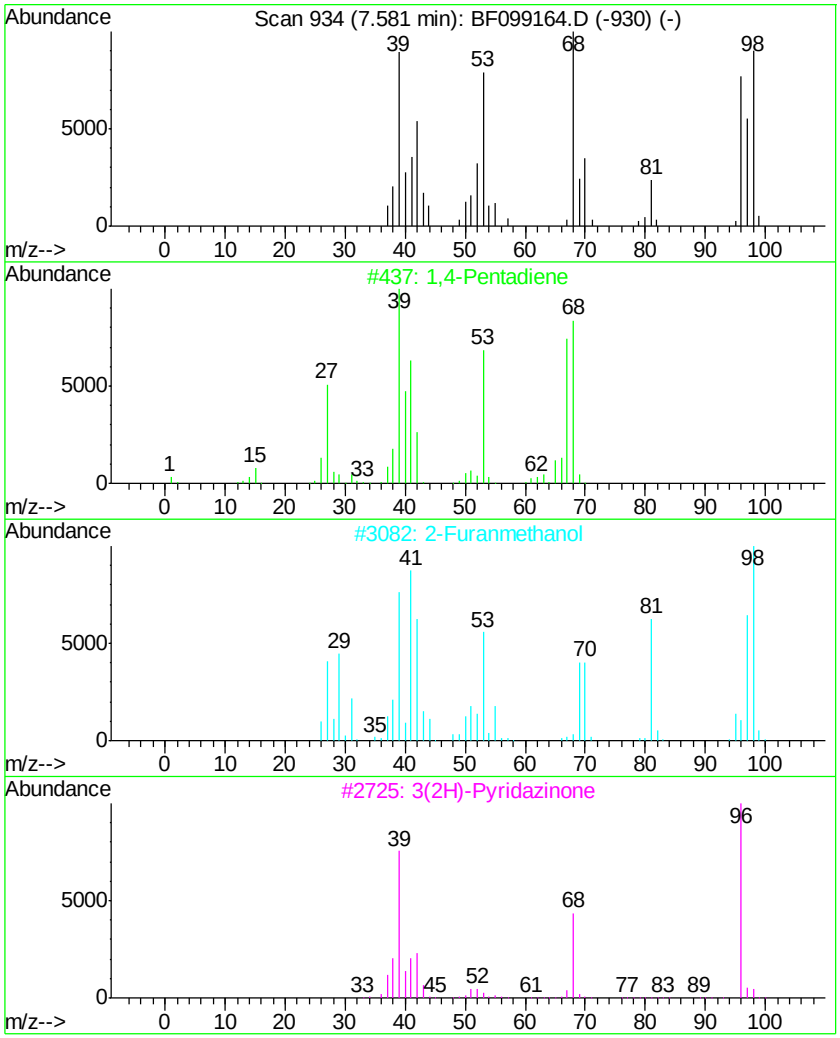
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

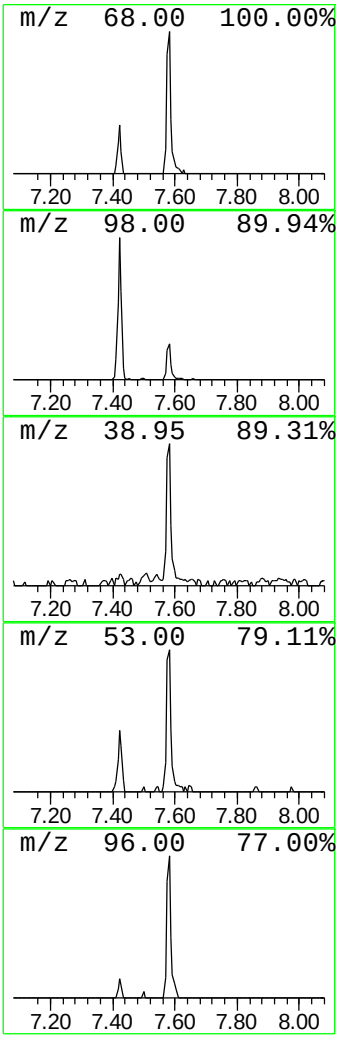
****

Peak Number 7 1,4-Pentadiene Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.58	2.19 ng	97441	Naphthalene-d8	8.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Pentadiene	68	C5H8	000591-93-5	64
2	2-Furanmethanol	98	C5H6O2	000098-00-0	64
3	3(2H)-Pyridazinone	96	C4H4N2O	000504-30-3	46
4	But-1-ene-3-yne, 1-ethoxy-	96	C6H8O	002806-41-9	45
5	2H-Pyran-2-one	96	C5H4O2	000504-31-4	43





Library Search Compound Report

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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

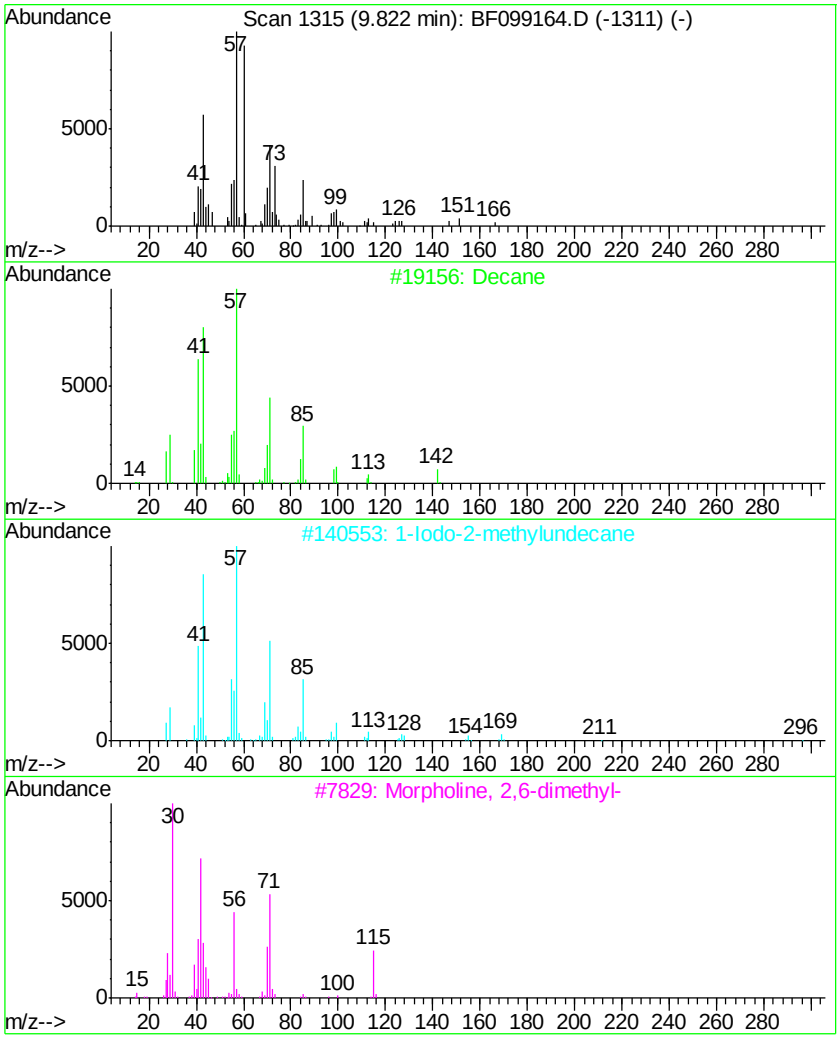
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

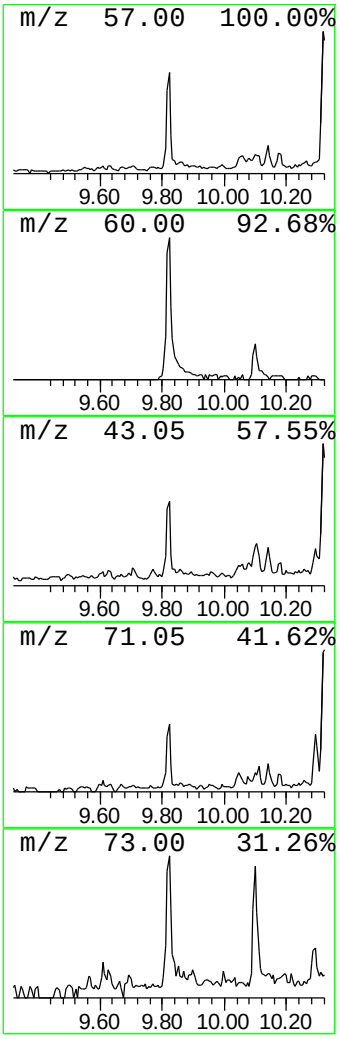
****

Peak Number 8 unknown9.82 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.82	2.24 ng	93008	Acenaphthene-d10	9.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decane	142	C10H22	000124-18-5	43
2	1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	30
3	Morpholine, 2,6-dimethyl-	115	C6H13NO	000141-91-3	30
4	Undecane, 3-methyl-	170	C12H26	001002-43-3	27
5	Undecane	156	C11H24	001120-21-4	27





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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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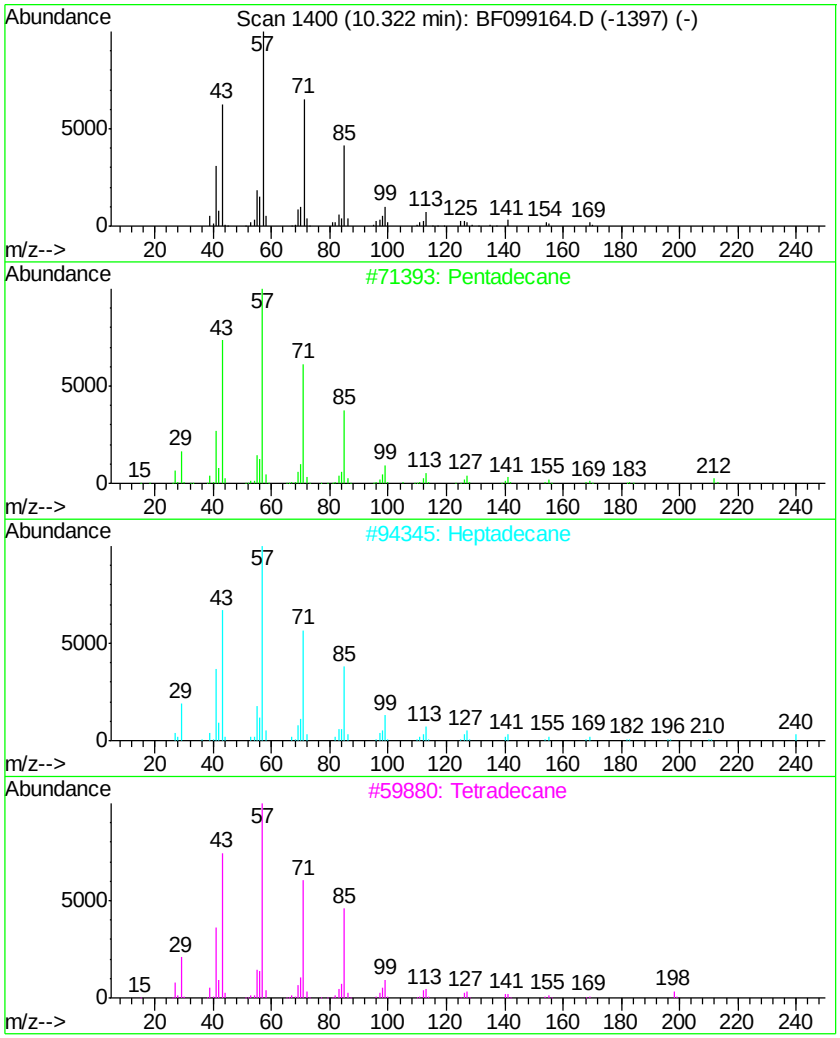
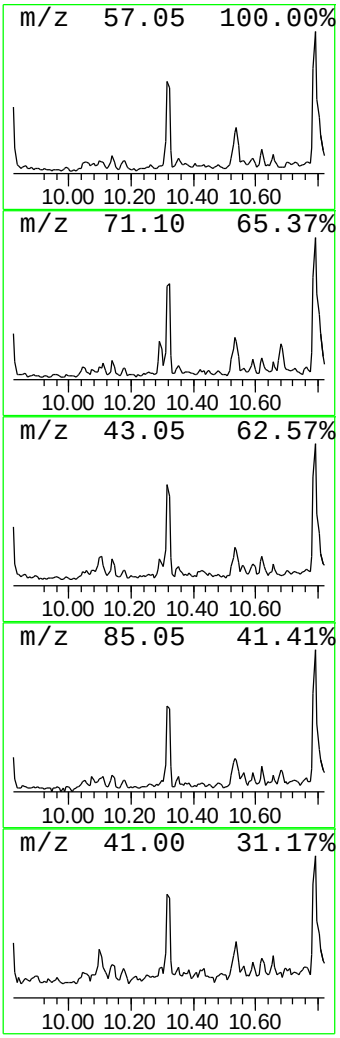
Peak Number 9 Pentadecane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.32	2.19 ng	90744	Acenaphthene-d10	9.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane	212	C15H32	000629-62-9	90
2	Heptadecane	240	C17H36	000629-78-7	86
3	Tetradecane	198	C14H30	000629-59-4	86
4	Tetratetracontane	619	C44H90	007098-22-8	83
5	Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	78





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Sample : I5516-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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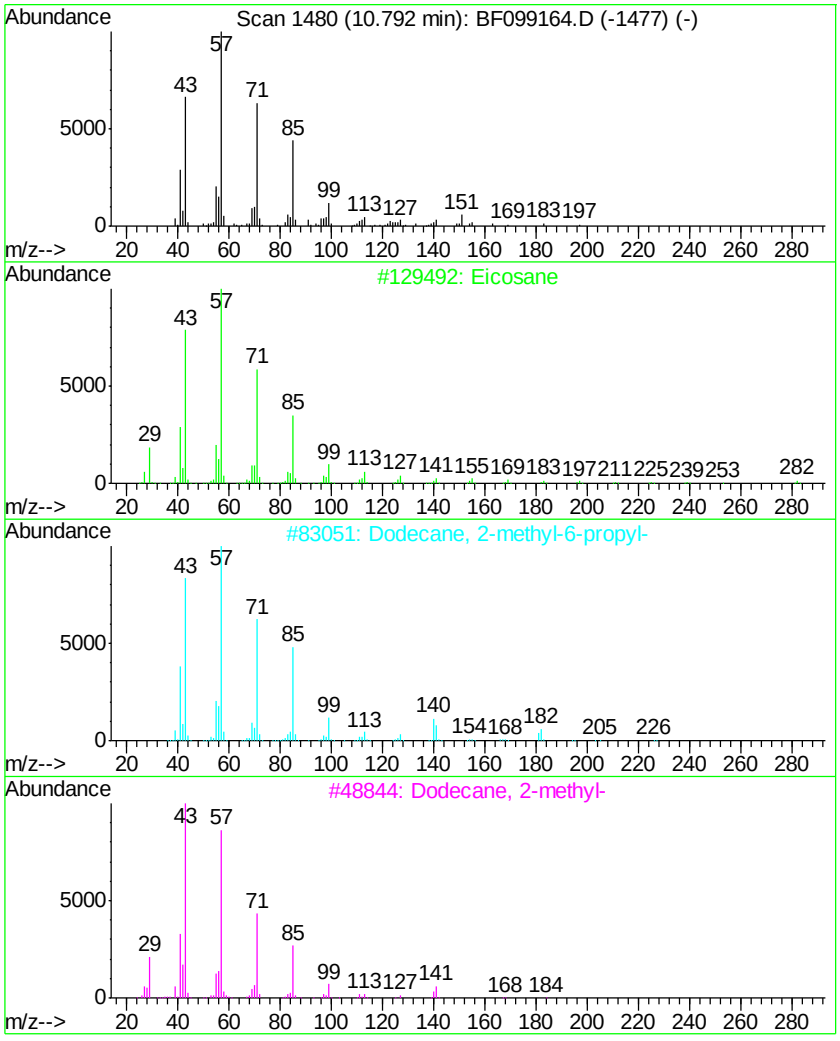
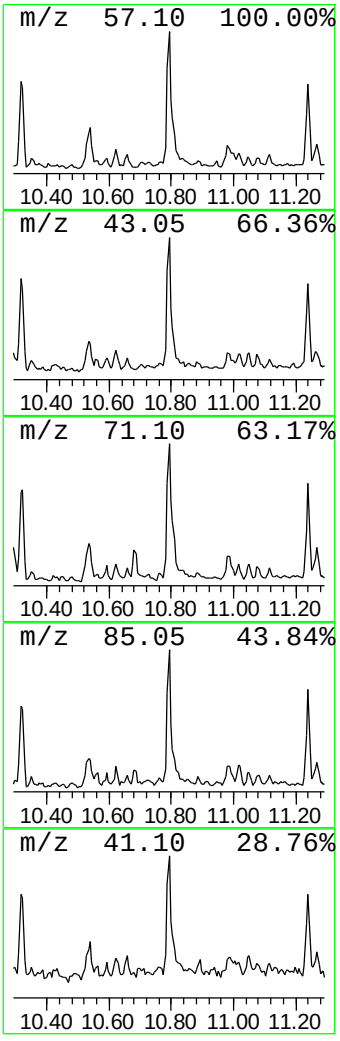
Peak Number 10 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.79	3.55 ng	173376	Phenanthrene-d10	11.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	80
2	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	80
3	Dodecane, 2-methyl-	184	C13H28	001560-97-0	80
4	Heneicosane	296	C21H44	000629-94-7	78
5	Bacchotricuneatin c	342	C20H22O5	066563-30-2	64





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Acq On : 6 Oct 2017 23:03
Operator : SJ/JU
Sample : I5516-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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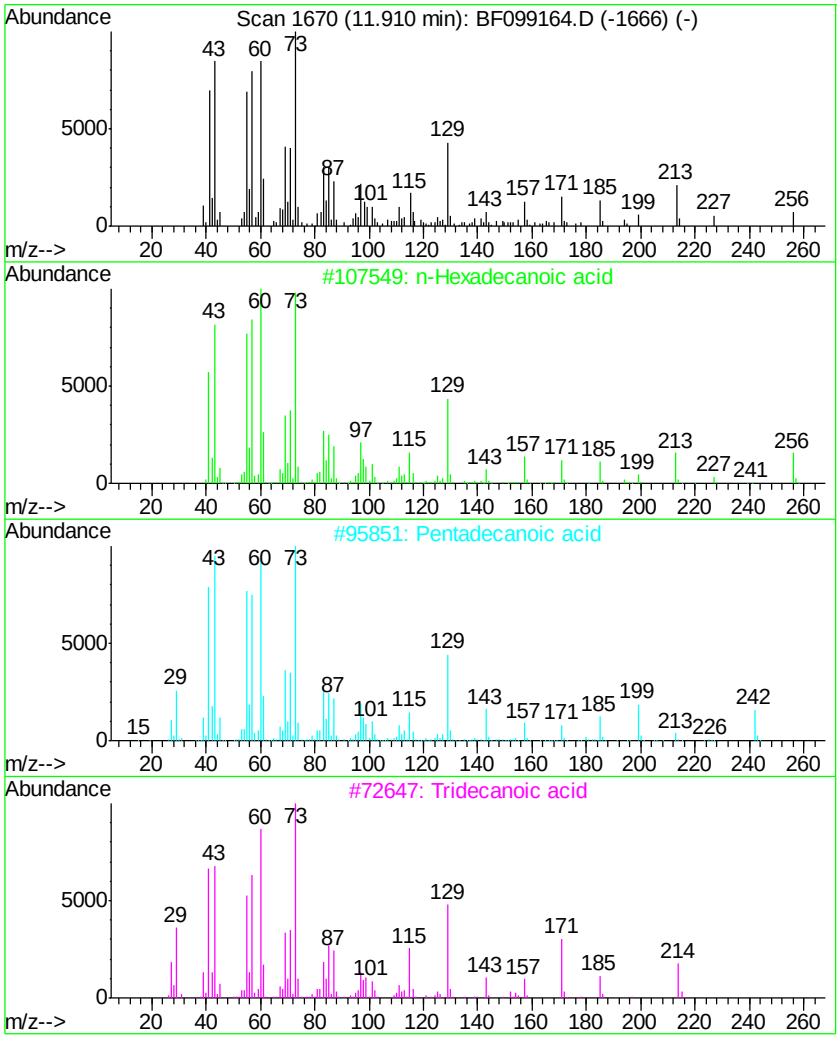
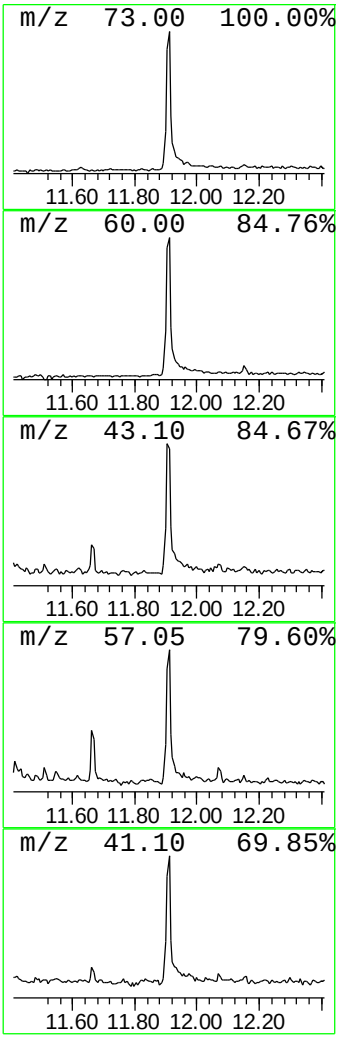
Peak Number 11 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.91	5.73 ng	279244	Phenanthrene-d10	11.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	Tridecanoic acid	214	C13H26O2	000638-53-9	91
4	n-Decanoic acid	172	C10H20O2	000334-48-5	76
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	64





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Data File : BF099164.D
Acq On : 6 Oct 2017 23:03
Operator : SJ/JU
Sample : I5516-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
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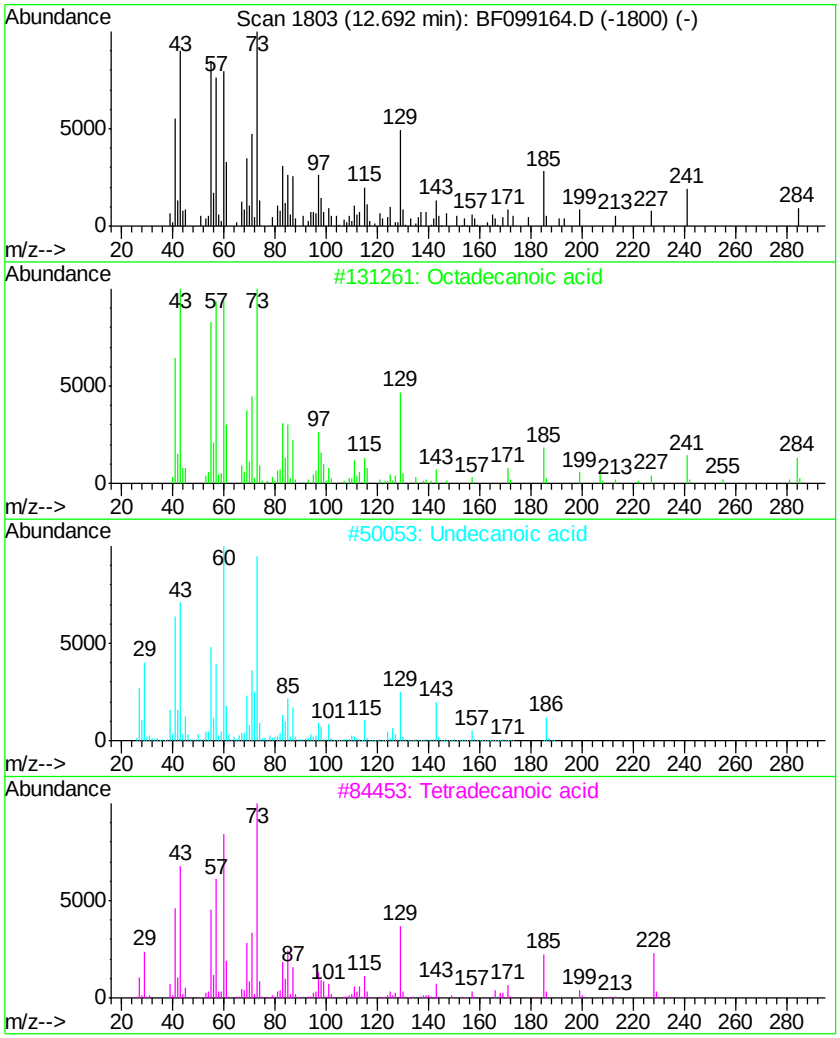
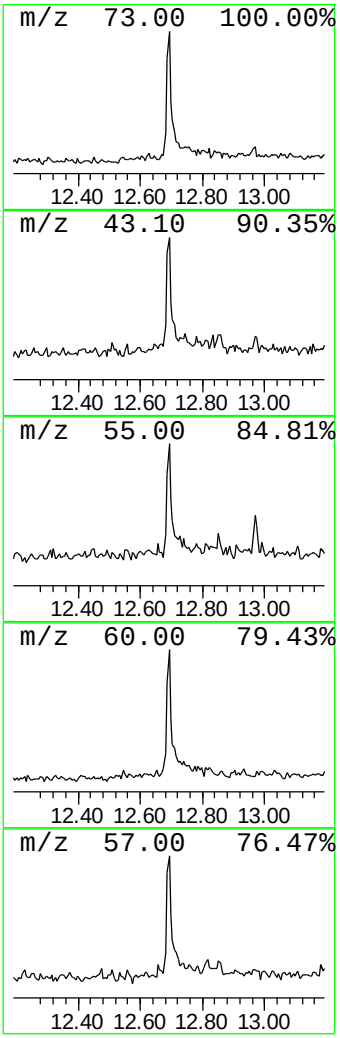
Peak Number 12 Octadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.69	2.50 ng	122107	Phenanthrene-d10	11.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	97
2	Undecanoic acid	186	C11H22O2	000112-37-8	74
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	68
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	46





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100617\
Data File : BF099164.D
Acq On : 6 Oct 2017 23:03
Operator : SJ/JU
Sample : I5516-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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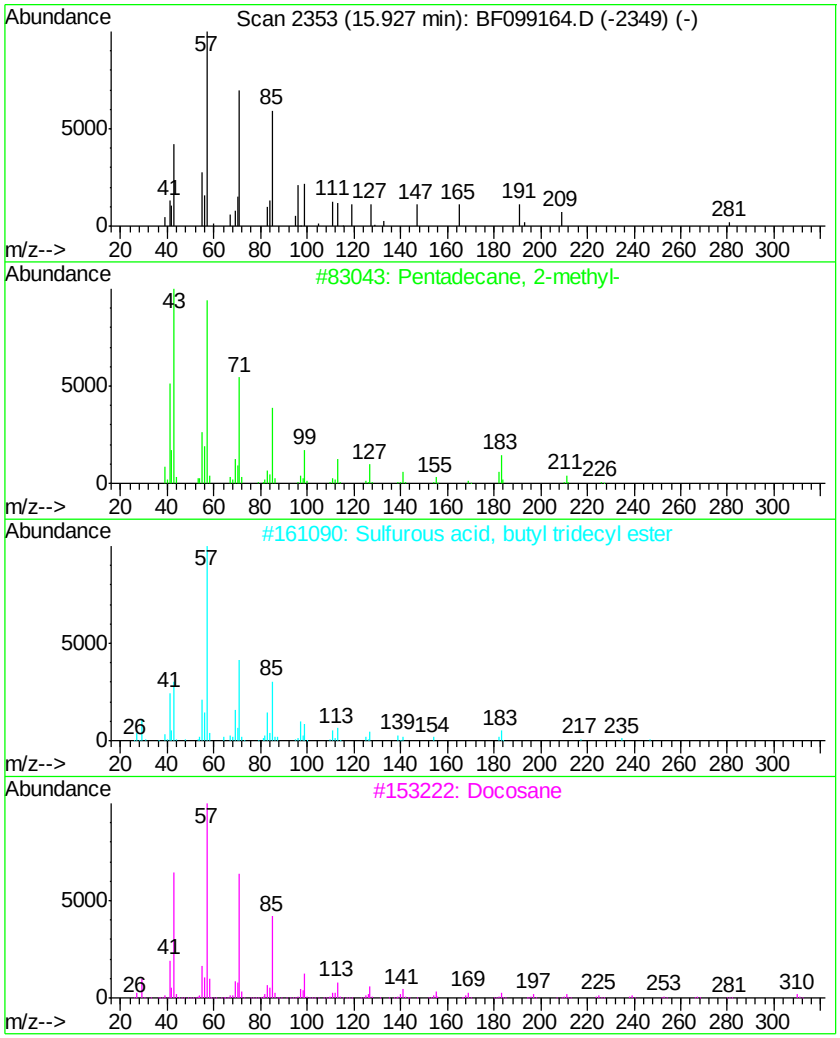
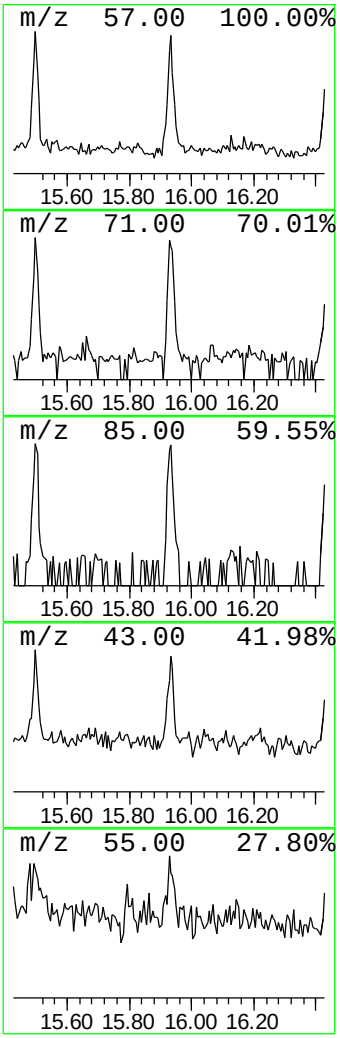
Peak Number 13 Pentadecane, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.93	3.32 ng	27044	Perylene-d12	15.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 2-methyl-	226	C16H34	001560-93-6	53
2	Sulfurous acid, butyl tridecyl e...	320	C17H36O3S	1000309-18-0	53
3	Docosane	310	C22H46	000629-97-0	50
4	Heneicosane	296	C21H44	000629-94-7	50
5	Octadecane	254	C18H38	000593-45-3	50





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100617\
Data File : BF099164.D
Acq On : 6 Oct 2017 23:03
Operator : SJ/JU
Sample : I5516-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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
Butane, 2-methoxy...	2.16	12.0	ng	392614	1	6.86	652551	20.0
4-Penten-2-one, 4...	3.61	6.9	ng	225766	1	6.86	652551	20.0
3-Penten-2-one, 4...	4.48	81.2	ng	2648510	1	6.86	652551	20.0
2-Pentanone, 4-hy...	5.08	4.7	ng	154049	1	6.86	652551	20.0
unknown6.63	6.63	30.3	ng	990075	1	6.86	652551	20.0
1,4-Pentadiene	7.58	2.2	ng	97441	2	8.15	890296	20.0
unknown9.82	9.82	2.2	ng	93008	3	9.90	829346	20.0
Pentadecane	10.32	2.2	ng	90744	3	9.90	829346	20.0
Eicosane	10.79	3.5	ng	173376	4	11.39	975480	20.0
n-Hexadecanoic acid	11.91	5.7	ng	279244	4	11.39	975480	20.0
Octadecanoic acid	12.69	2.5	ng	122107	4	11.39	975480	20.0
Pentadecane, 2-me...	15.93	3.3	ng	27044	6	15.49	163076	20.0