LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF030117\
Data File : BF093305.D
Acq On : 1 Mar 2017 22:36
Operator : SJ/MA
Sample : I2012-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P-9

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	3.001	77	80	91	rBV	45522	146262	1.23%	0.381%
2	3.230	97	100	112	rVB	178834	375545	3.16%	0.979%
3	4.304	188	194	196	rBV	5279686	11866145	100.00%	30.920%
4	4.978	249	253	256	rBV	3493208	7654260	64.51%	19.945%
5	6.464	381	383	389	rBV	71545	124440	1.05%	0.324%
6	6.807	410	413	415	rBV	626783	896737	7.56%	2.337%
7	6.956	424	426	429	rBV	2112932	1934730	16.30%	5.041%
8	7.139	439	442	446	rBV	162894	223956	1.89%	0.584%
9	7.367	460	462	465	rBV	1182874	1517329	12.79%	3.954%
10	8.087	523	525	528	rBV	1219871	1164803	9.82%	3.035%
11	9.162	617	619	622	rBV	2461008	2690142	22.67%	7.010%
12	9.562	652	654	658	rBV	282755	296672	2.50%	0.773%
13	9.847	676	679	681	rBV	933442	1338802	11.28%	3.489%
14	10.739	756	757	762	rBV3	96627	189208	1.59%	0.493%
15	10.842	765	766	768	rVV2	114466	136952	1.15%	0.357%
16	10.876	768	769	773	rVV	82628	139427	1.17%	0.363%
17	11.025	781	782	785	rVV2	71700	119571	1.01%	0.312%
18	11.185	794	796	802	rBV3	73522	151755	1.28%	0.395%
19	11.322	806	808	814	rBV	1013890	1471577	12.40%	3.834%
20	11.893	855	858	860	rBV	290004	398970	3.36%	1.040%
21	12.545	913	915	917	rBV	145753	152498	1.29%	0.397%
22	12.773	932	935	937	rVB	96641	137353	1.16%	0.358%
23	12.911	944	947	950	rBV	2550383	2519747	21.23%	6.566%
24	13.802	1021	1025	1030	rBV	181200	316006	2.66%	0.823%
25	13.974	1037	1040	1042	rBV	765130	1102401	9.29%	2.873%
26	14.705	1102	1104	1108	rBV2	199416	307839	2.59%	0.802%
27	15.391	1161	1164	1167	rBV	707045	874914	7.37%	2.280%
28	16.797	1284	1287	1291	rBV3	52288	129359	1.09%	0.337%

Sum of corrected areas: 38377400

LSC Report - Integrated Chromatogram

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Operator : SJ/MA
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Misc :
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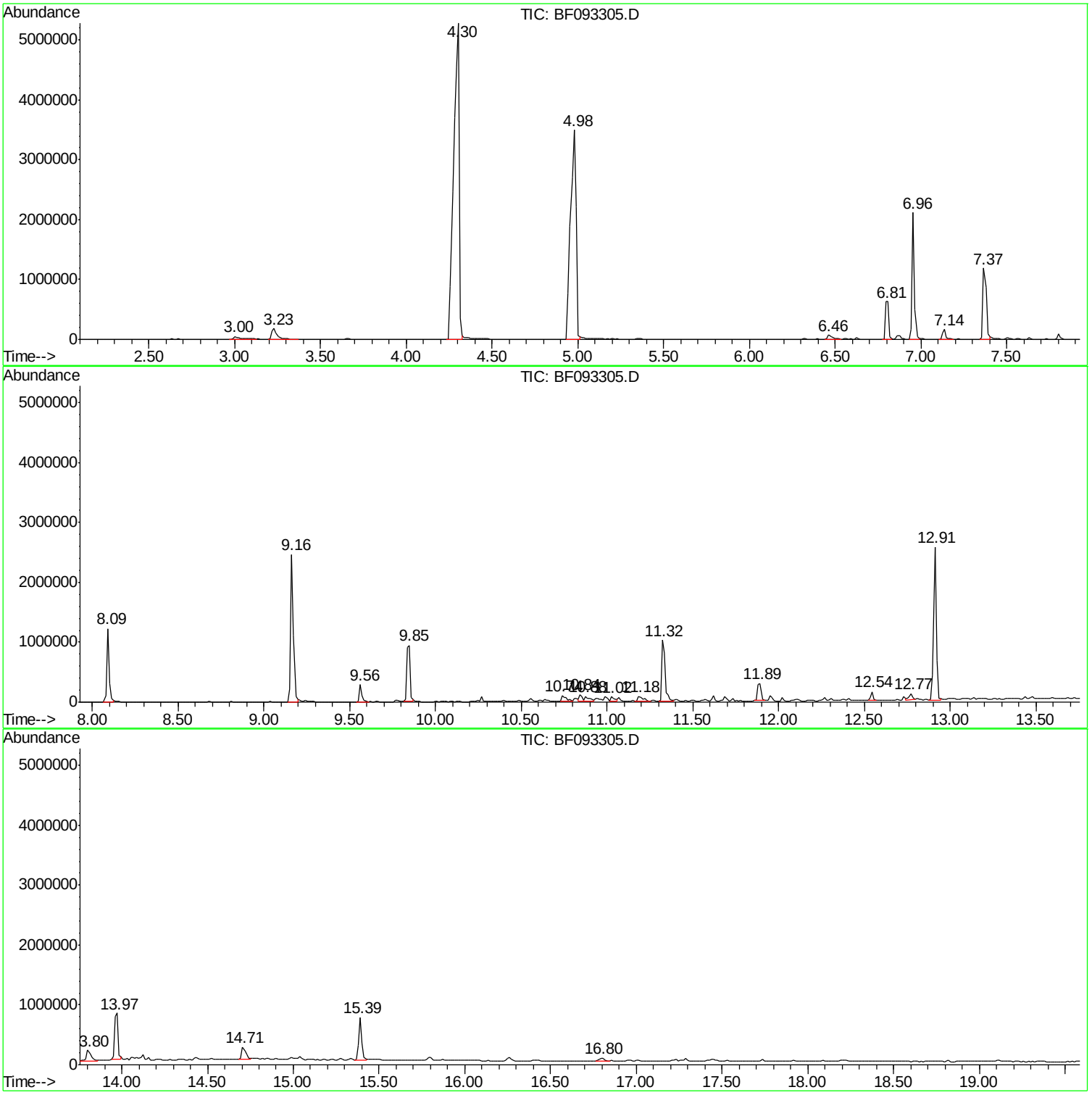
Instrument : BNA_F
ClientSampleId : P-9

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\BF030117\
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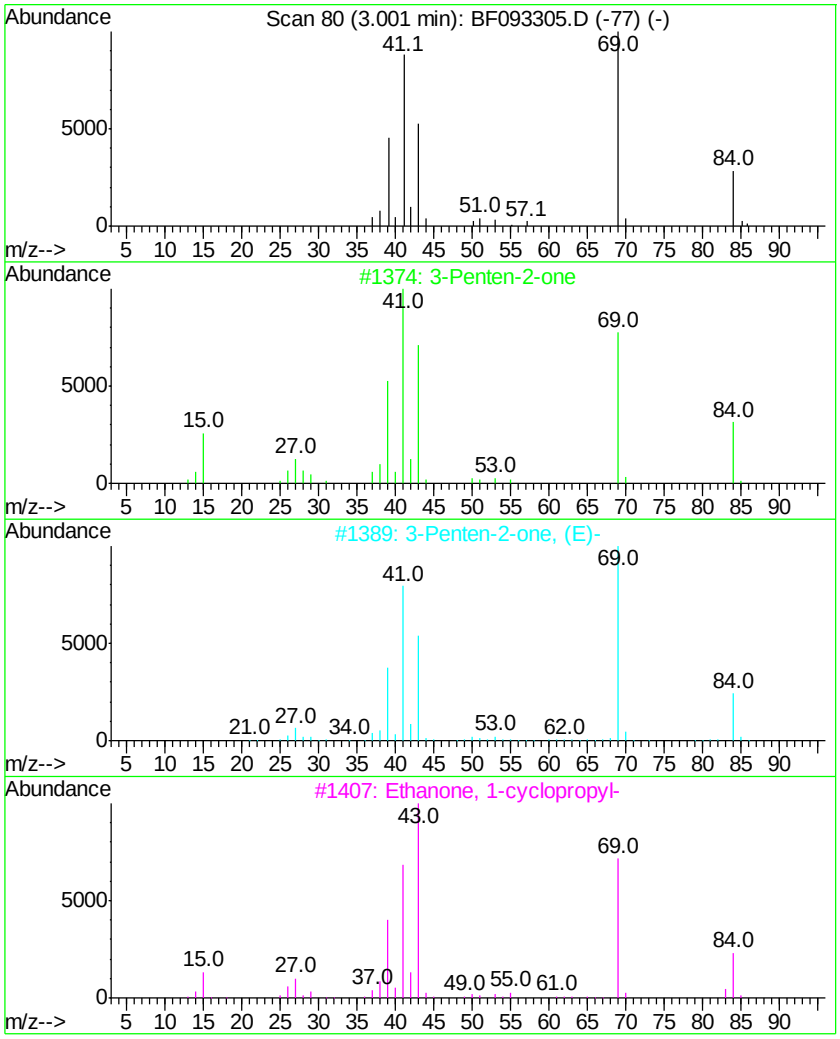
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

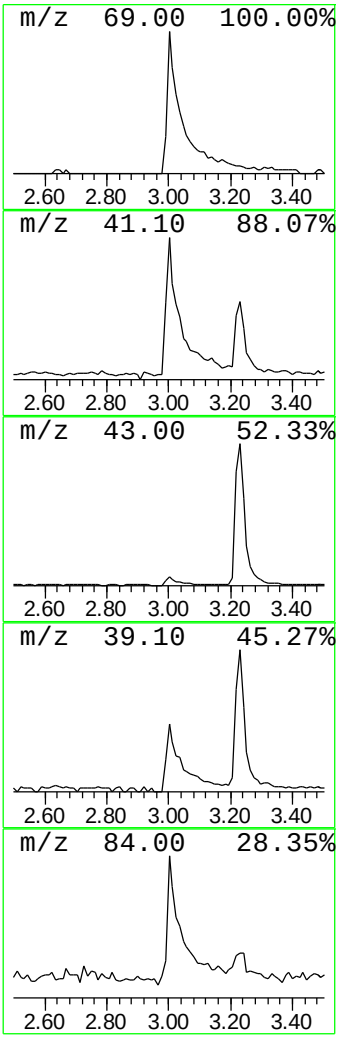
****

Peak Number 1 3-Penten-2-one Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.00	3.26 ng	146262	1,4-Dichlorobenzene-d4	6.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one	84	C5H8O	000625-33-2	91
2	3-Penten-2-one, (E)-	84	C5H8O	003102-33-8	76
3	Ethanone, 1-cyclopropyl-	84	C5H8O	000765-43-5	72
4	2-Pentene, 4-methyl-, (Z)-	84	C6H12	000691-38-3	64
5	2-Butene, 2,3-dimethyl-	84	C6H12	000563-79-1	64





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ClientSampleId : P-9

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

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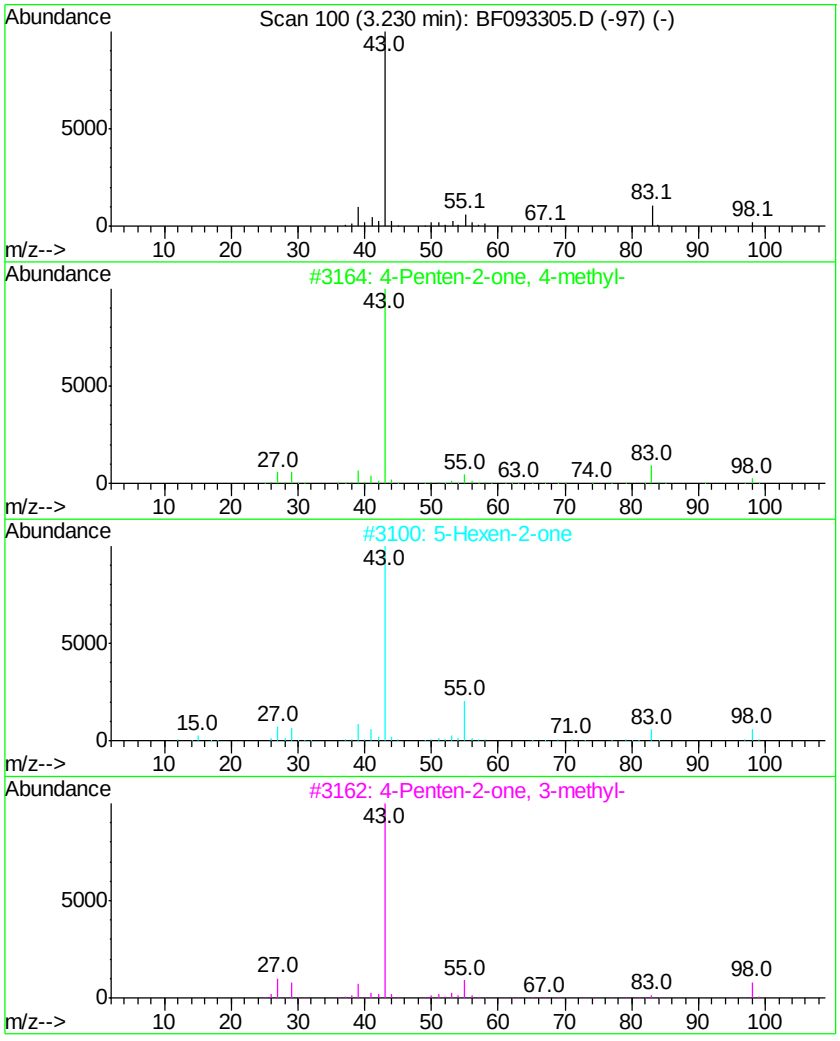
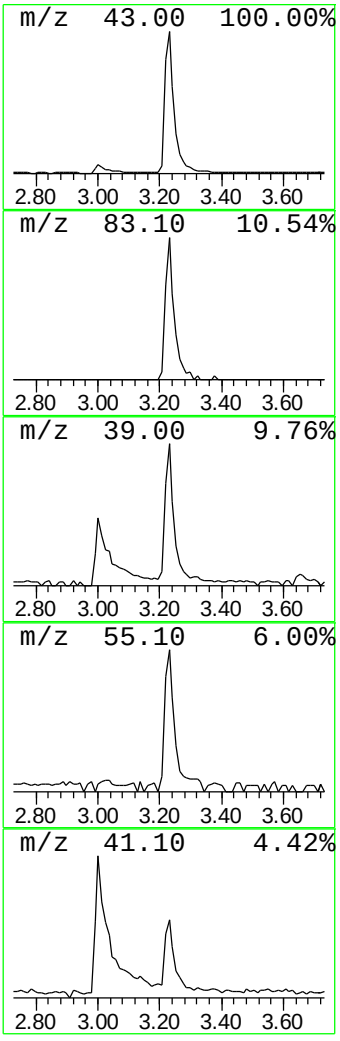
Peak Number 2 4-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.23	8.38 ng	375545	1,4-Dichlorobenzene-d4	6.81

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	37
3	4-Penten-2-one, 3-methyl-	98	C6H10O	000758-87-2	9
4	Methyl 1-methylcyclopropyl ketone	98	C6H10O	001567-75-5	9
5	4-Hexen-2-one	98	C6H10O	025659-22-7	9





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Operator : SJ/MA
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Misc :
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Instrument : BNA_F
ClientSampleId : P-9

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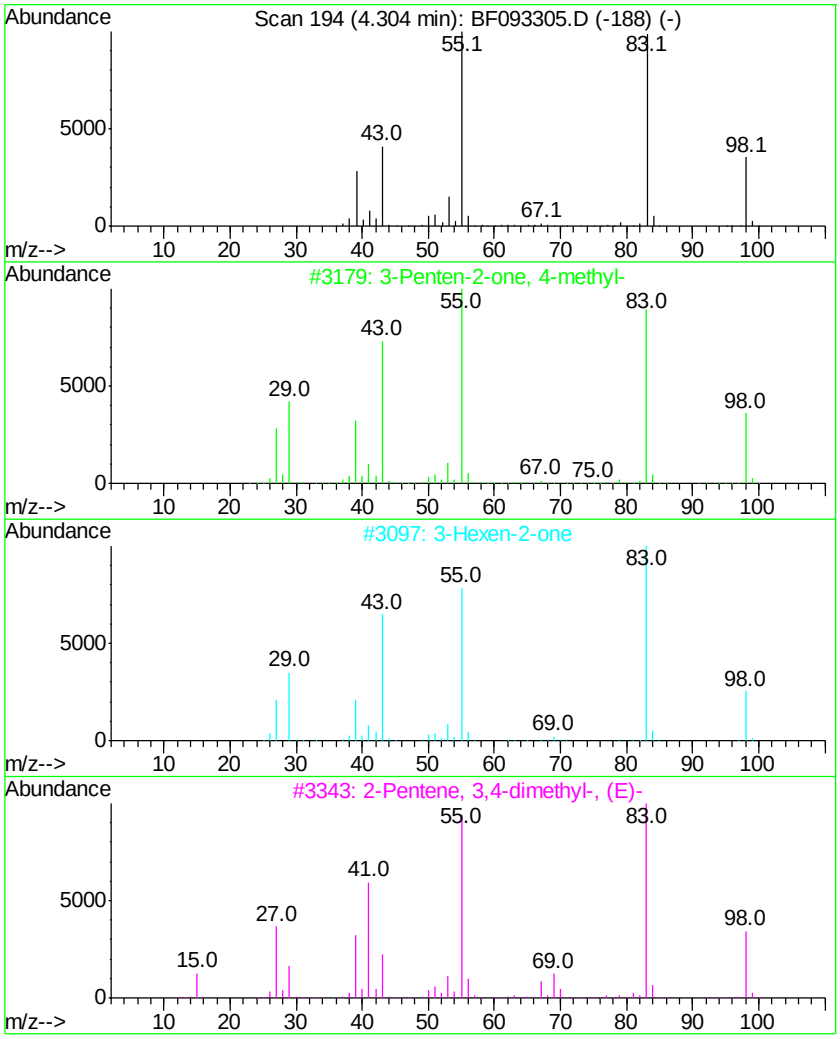
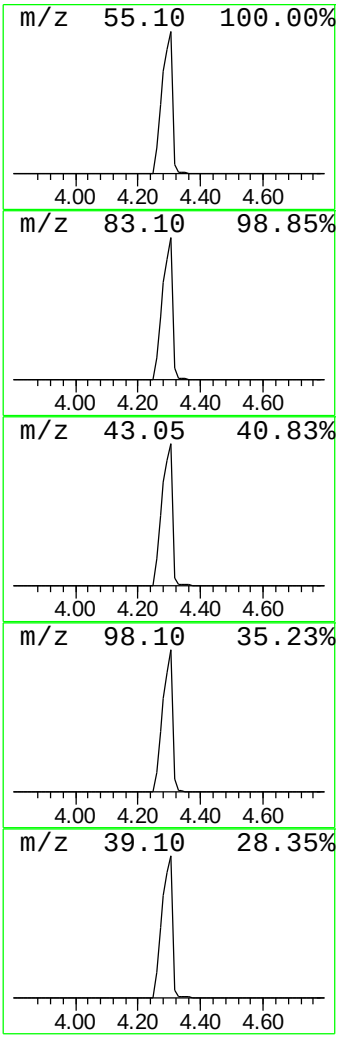
Peak Number 3 3-Penten-2-one, 4-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.30	264.65 ng	11866100	1,4-Dichlorobenzene-d4	6.81

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-, (E)-	98	C7H14	004914-92-5	90
4	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
5	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86





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Sample : I2012-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P-9

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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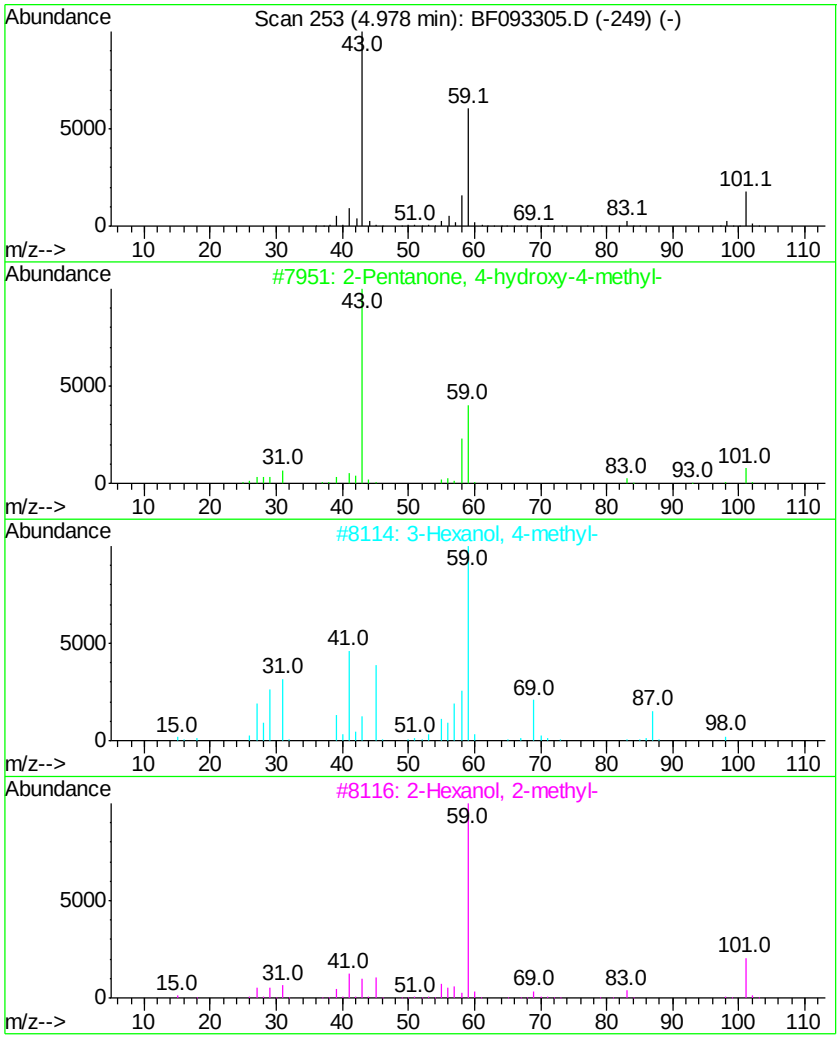
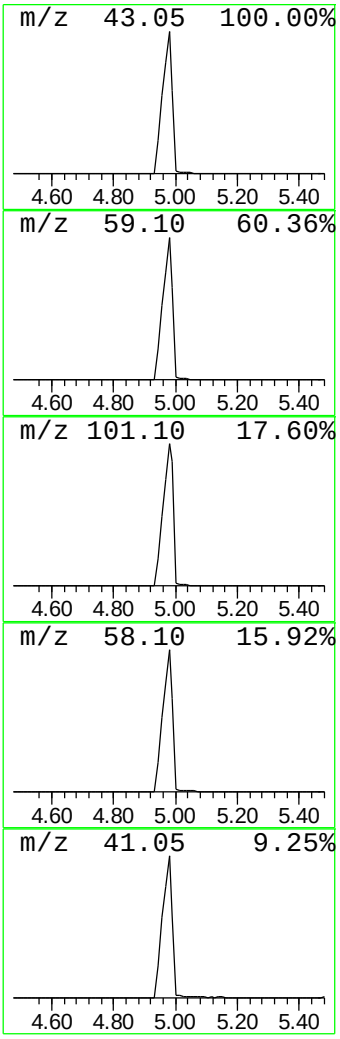
Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.98	170.71 ng	7654260	1,4-Dichlorobenzene-d4	6.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25





Data Path : Z:\HPCHEM1\BNA F\DATA\BF030117\
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Sample : I2012-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P-9

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
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TIC Library : C:\DATABASE\NIST02.L
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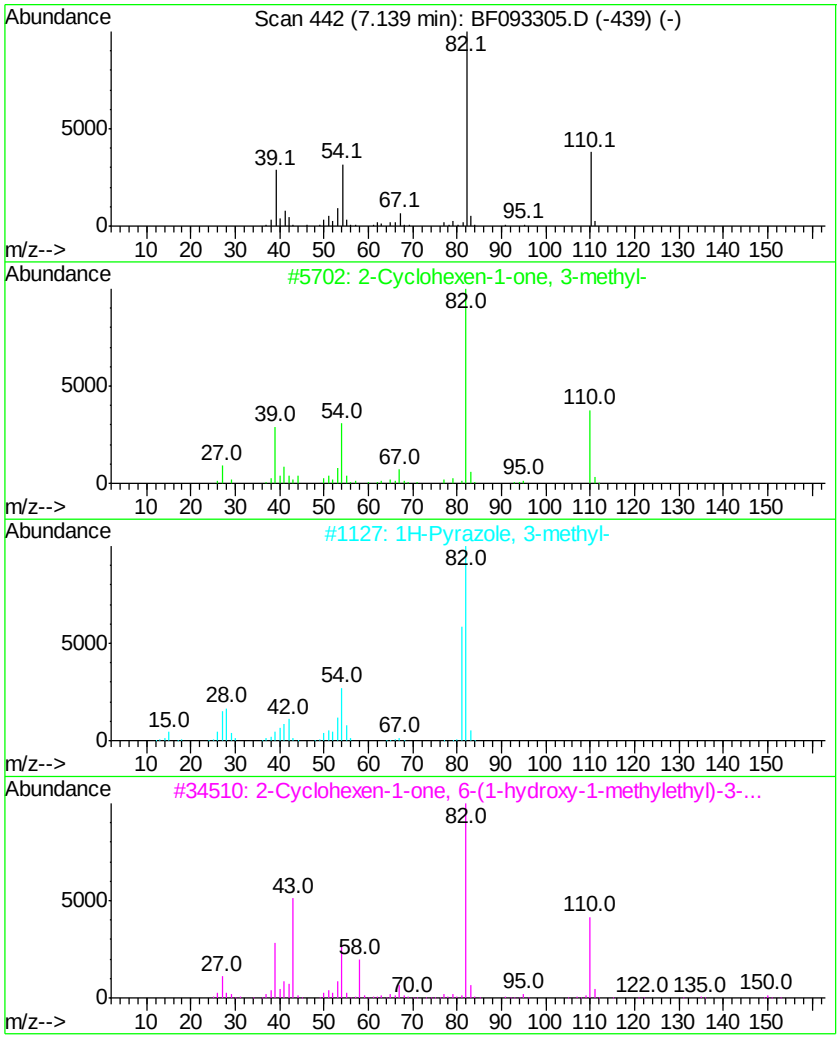
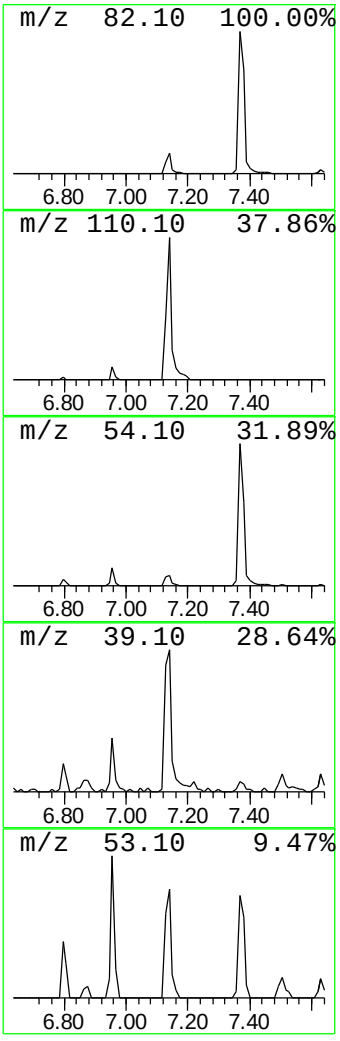
Peak Number 6 2-Cyclohexen-1-one, 3-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.14	4.99 ng	223956	1,4-Dichlorobenzene-d4	6.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Cyclohexen-1-one, 3-methyl-	110	C7H10O	001193-18-6	91
2	1H-Pyrazole, 3-methyl-	82	C4H6N2	001453-58-3	45
3	2-Cyclohexen-1-one, 6-(1-hydroxy...	168	C10H16O2	087791-00-2	43
4	Betazole	111	C5H9N3	000105-20-4	40
5	1H-Imidazole, 4-methyl-	82	C4H6N2	000822-36-6	36





Library Search Compound Report

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Instrument : BNA_F
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TIC Library : C:\DATABASE\NIST02.L
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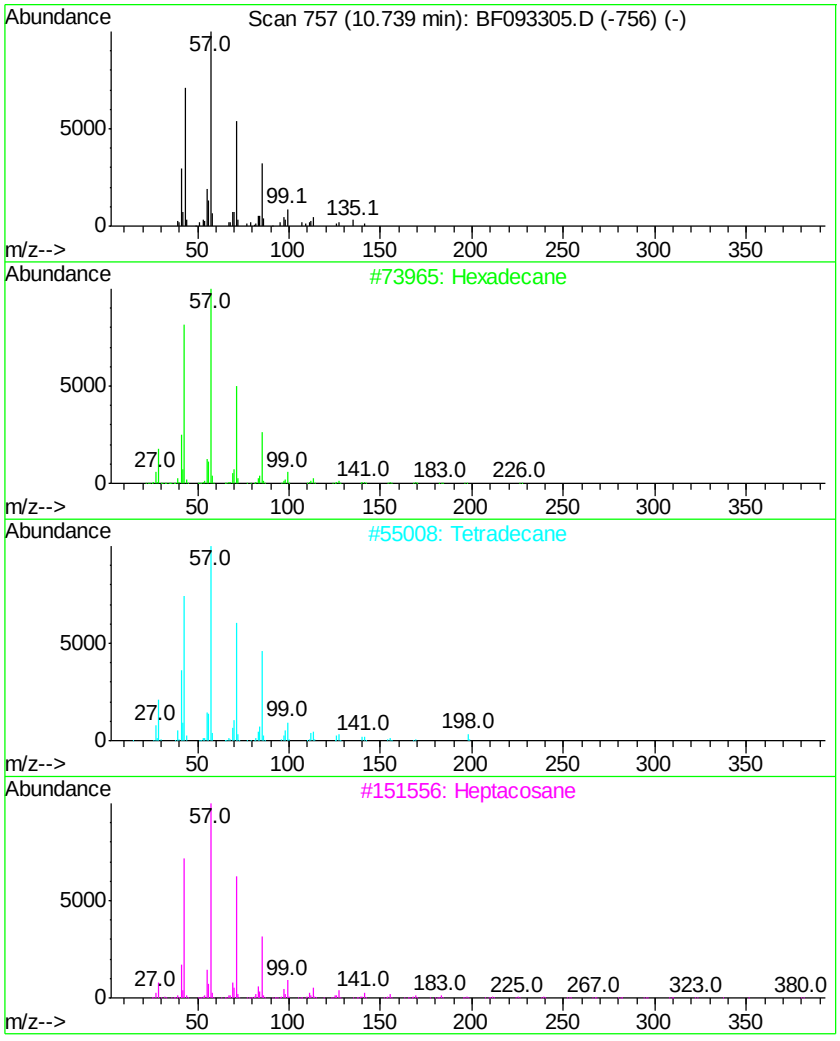
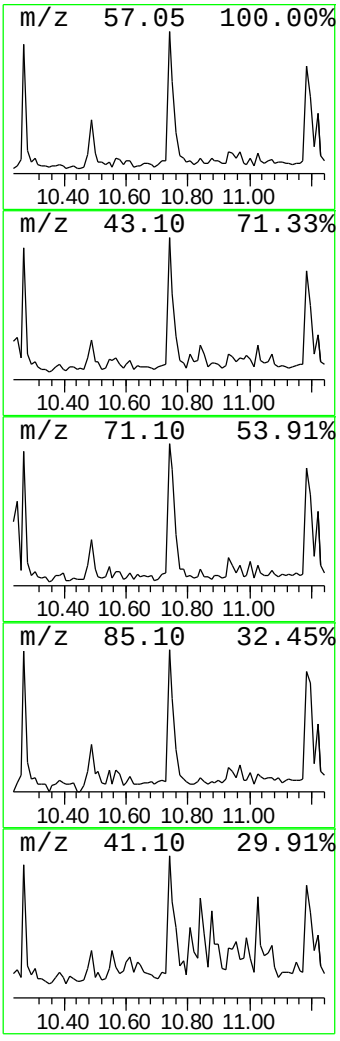
Peak Number 7 Hexadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.74	2.57 ng	189208	Phenanthrene-d10	11.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	90
2	Tetradecane	198	C14H30	000629-59-4	86
3	Heptacosane	380	C27H56	000593-49-7	86
4	Pentadecane	212	C15H32	000629-62-9	86
5	Eicosane	282	C20H42	000112-95-8	78





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

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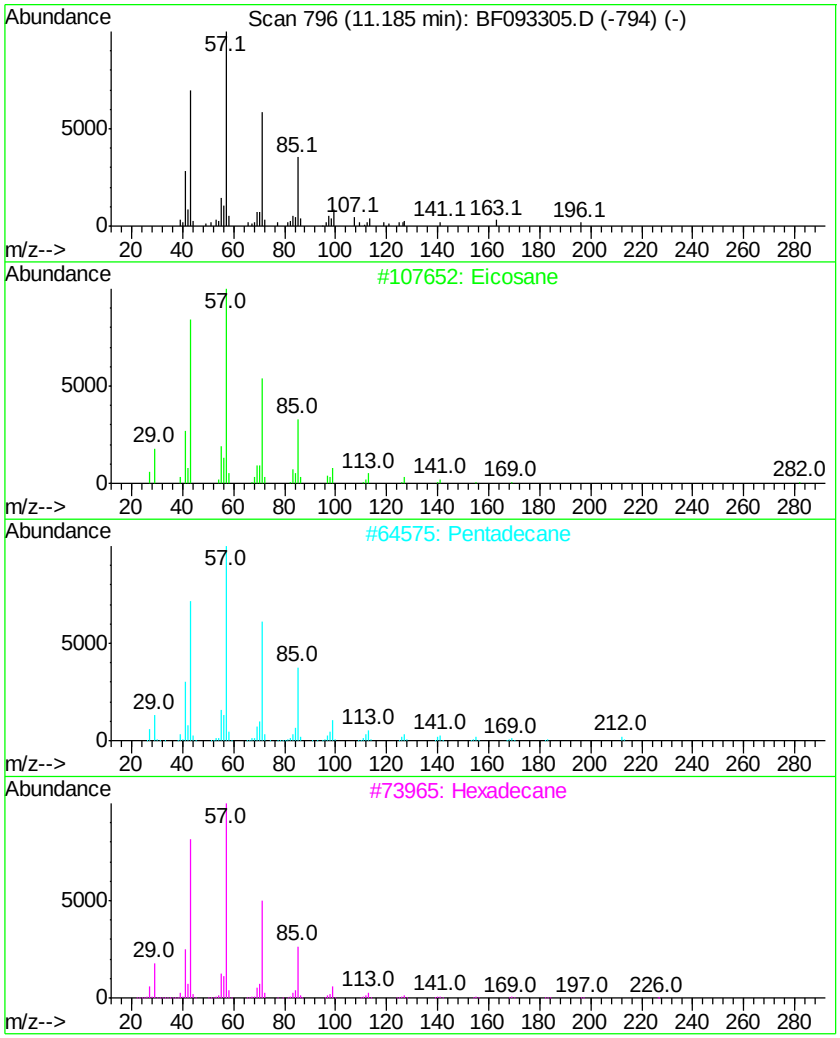
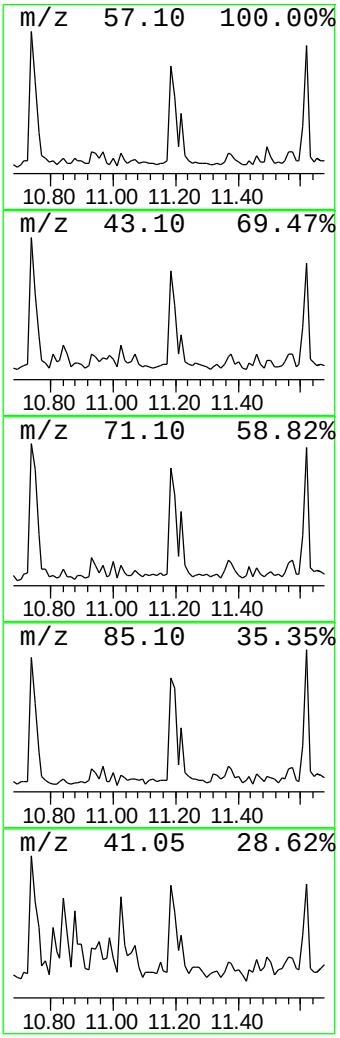
Peak Number 8 Eicosane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.18	2.06 ng	151755	Phenanthrene-d10	11.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	90
2	Pentadecane	212	C15H32	000629-62-9	80
3	Hexadecane	226	C16H34	000544-76-3	80
4	Heptadecane, 8-methyl-	254	C18H38	013287-23-5	72
5	Octadecane	254	C18H38	000593-45-3	72





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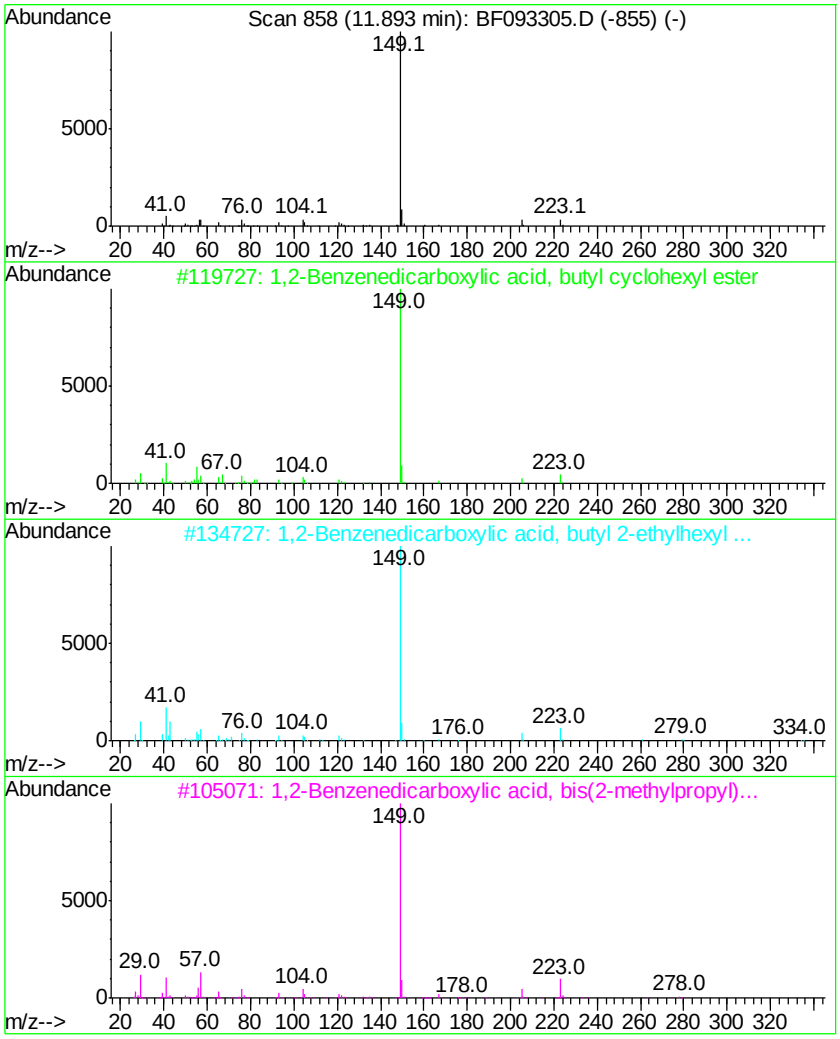
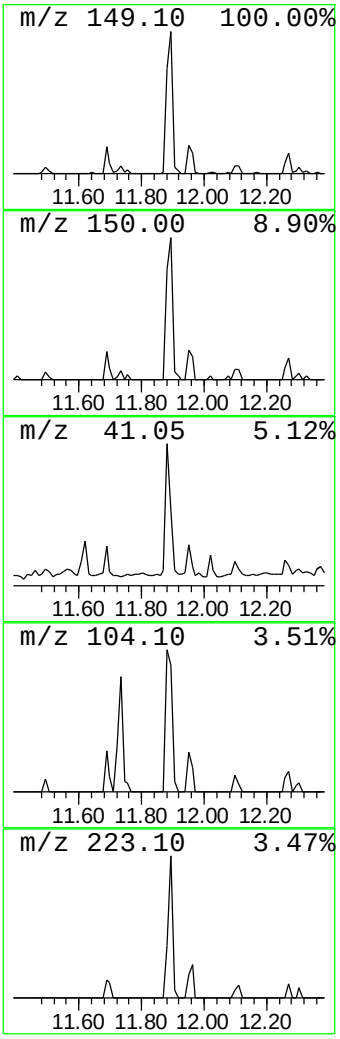
Peak Number 9 1,2-Benzenedicarboxylic aci... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.89	5.42 ng	398970	Phenanthrene-d10	11.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Benzenedicarboxylic acid, bu...	304	C18H24O4	000084-64-0	90
2	1,2-Benzenedicarboxylic acid, bu...	334	C20H30O4	000085-69-8	83
3	1,2-Benzenedicarboxylic acid, bi...	278	C16H22O4	000084-69-5	83
4	1,2-Benzenedicarboxylic acid, bu...	334	C20H30O4	000084-78-6	83
5	1,2-Benzenedicarboxylic acid, bu...	362	C22H34O4	000089-19-0	74





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

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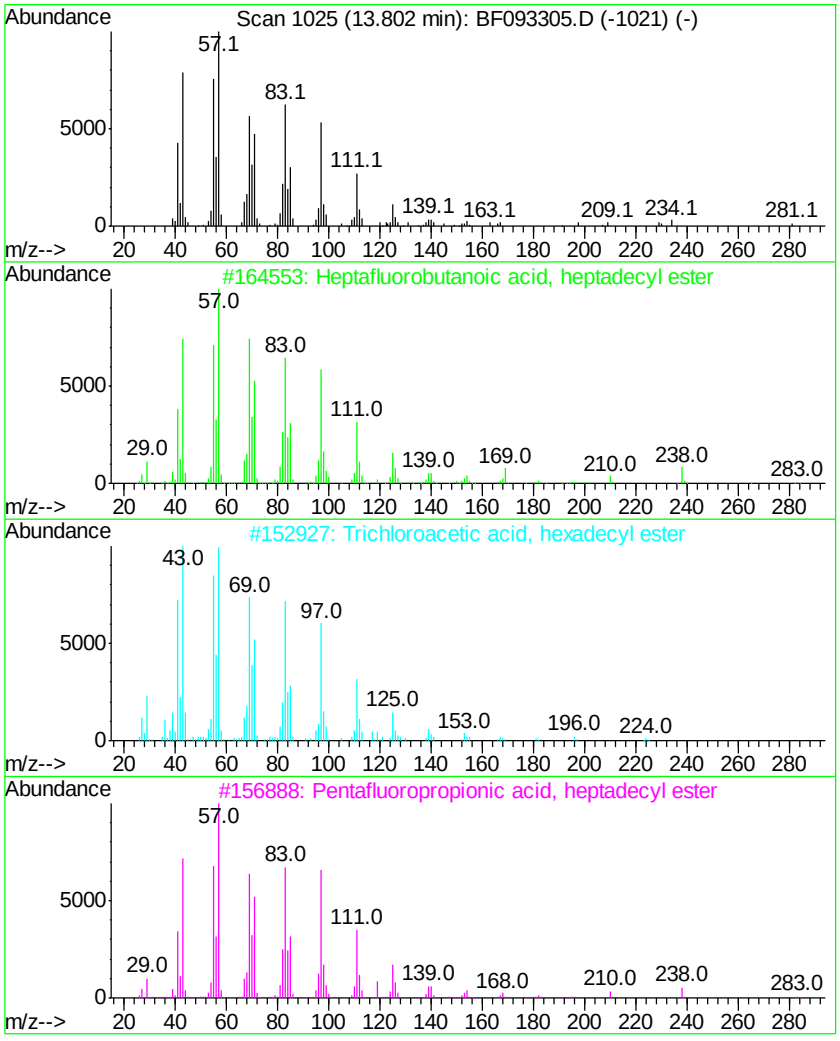
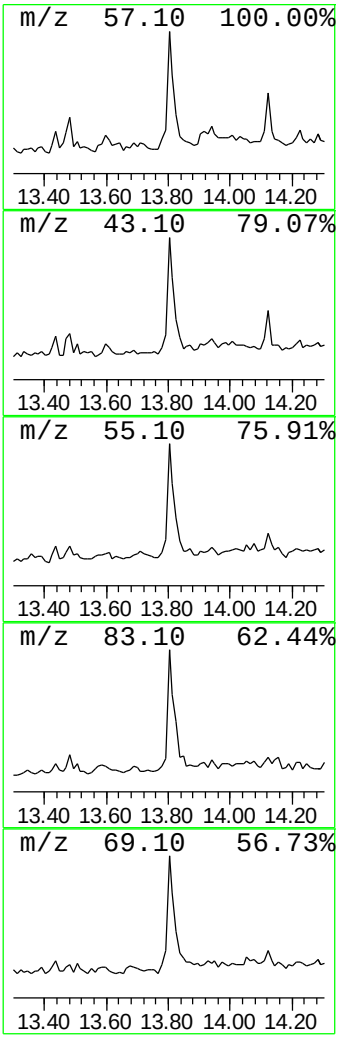
Peak Number 12 Heptafluorobutanoic acid, h... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.80	5.73 ng	316006	Chrysene-d12	13.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	94
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
3	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	91
4	17-Pentatriacontene	491	C35H70	006971-40-0	91
5	Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	90





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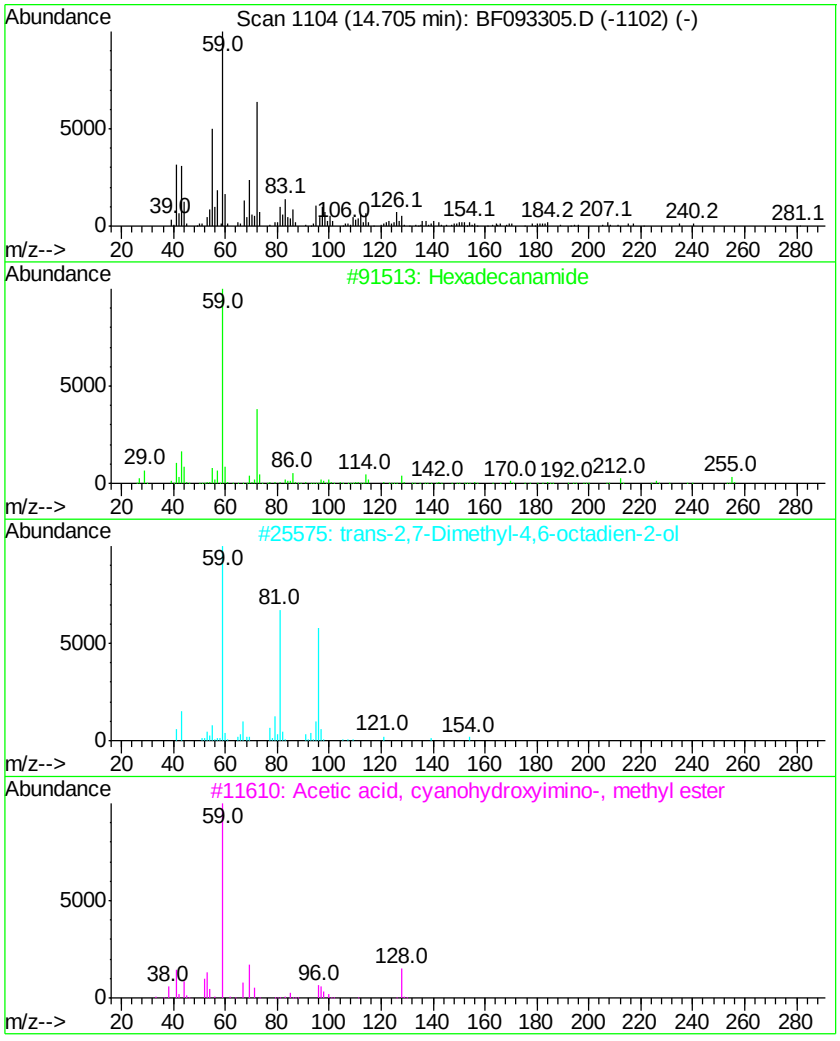
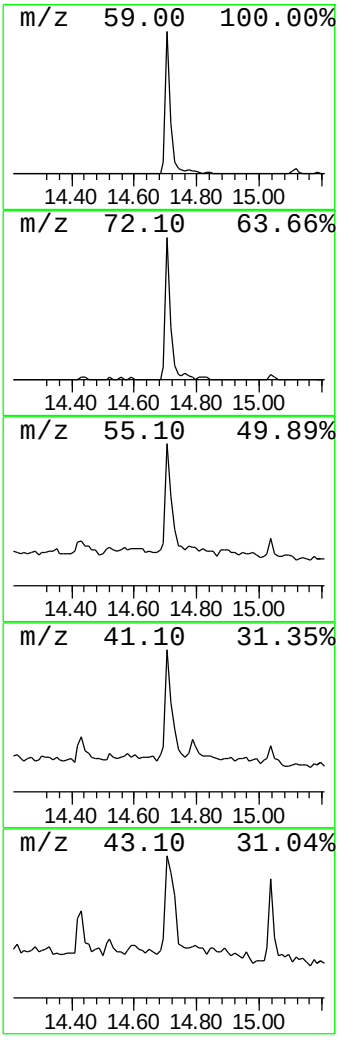
****

Peak Number 13 Hexadecanamide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.71	7.04 ng	307839	Perylene-d12	15.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanamide	255	C16H33NO	000629-54-9	72
2	trans-2,7-Dimethyl-4,6-octadien-...	154	C10H18O	1000281-69-5	47
3	Acetic acid, cyanohydroxyimino-,...	128	C4H4N2O3	061295-92-9	43
4	Decanamide-	171	C10H21NO	002319-29-1	40
5	2-Methyl-tridecane-2,12-diol	230	C14H30O2	1000187-03-5	38





Data Path : Z:\HPCHEM1\BNA F\DATA\BF030117\
Data File : BF093305.D
Acq On : 1 Mar 2017 22:36
Operator : SJ/MA
Sample : I2012-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P-9

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

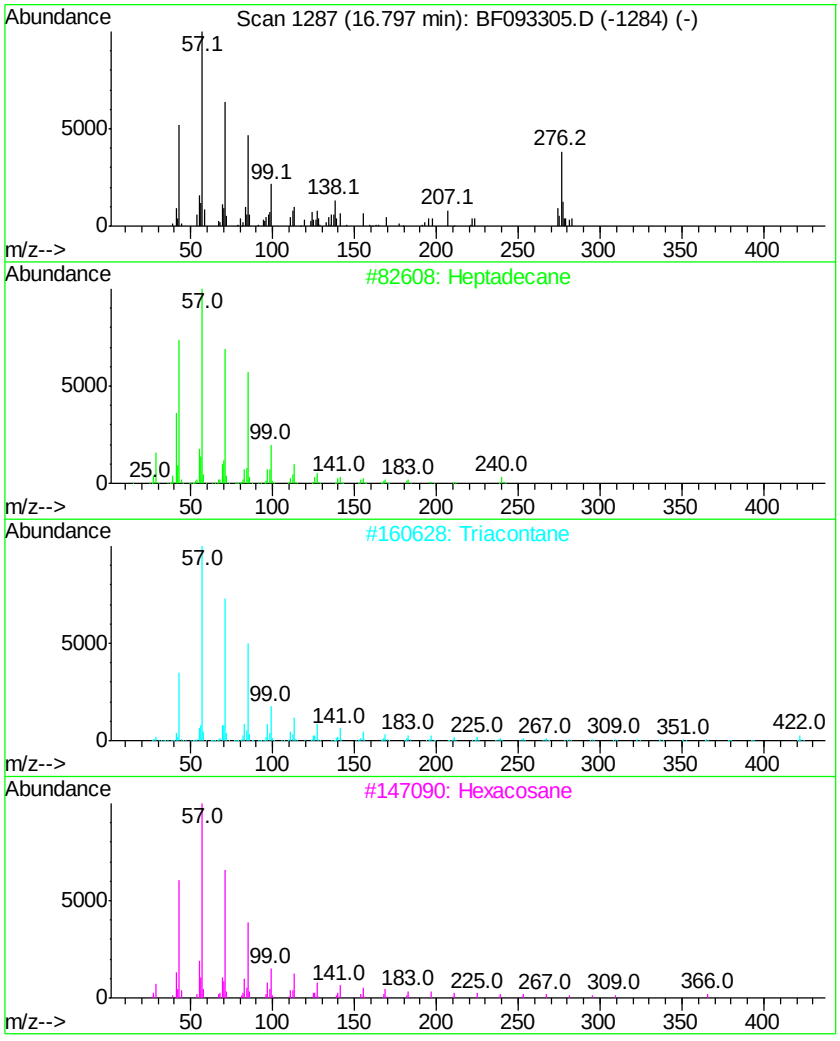
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

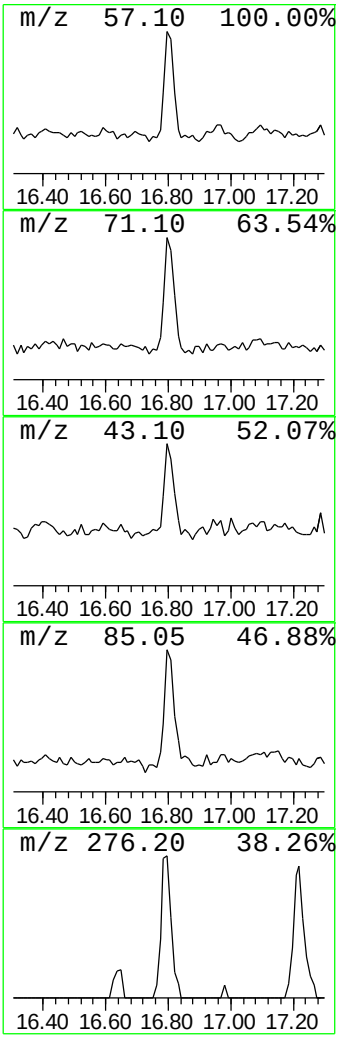
****

Peak Number 14 unknown16.80 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.80	2.96 ng	129359	Perylene-d12	15.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	49
2	Triacontane	422	C30H62	000638-68-6	49
3	Hexacosane	366	C26H54	000630-01-3	49
4	Pentacosane	352	C25H52	000629-99-2	49
5	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	46





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030117\
Data File : BF093305.D
Acq On : 1 Mar 2017 22:36
Operator : SJ/MA
Sample : I2012-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P-9

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
3-Penten-2-one	3.00	3.3	ng	146262	1	6.81	896737	20.0
4-Penten-2-one, 4...	3.23	8.4	ng	375545	1	6.81	896737	20.0
3-Penten-2-one, 4...	4.30	264.6	ng	11866100	1	6.81	896737	20.0
2-Pentanone, 4-hy...	4.98	170.7	ng	7654260	1	6.81	896737	20.0
2-Cyclohexen-1-on...	7.14	5.0	ng	223956	1	6.81	896737	20.0
Hexadecane	10.74	2.6	ng	189208	4	11.32	1471580	20.0
Eicosane	11.18	2.1	ng	151755	4	11.32	1471580	20.0
1,2-Benzenedicarb...	11.89	5.4	ng	398970	4	11.32	1471580	20.0
Heptafluorobutano...	13.80	5.7	ng	316006	5	13.97	1102400	20.0
Hexadecanamide	14.71	7.0	ng	307839	6	15.39	874914	20.0
unknown16.80	16.80	3.0	ng	129359	6	15.39	874914	20.0