LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF122217\
Data File : BF101674.D
Acq On : 23 Dec 2017 00:37
Operator : SJ/JU
Sample : I6957-01
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HALSTED-NW

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-BF121417.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	3.452	226	232	256	rBV	541214	1106182	4.39%	1.707%
2	4.440	383	400	403	rBV	5785354	25171174	100.00%	38.846%
3	5.046	491	503	505	rBV	3782644	9411558	37.39%	14.525%
4	5.740	618	621	629	rBV	188090	269452	1.07%	0.416%
5	6.787	796	799	807	rBV	999976	937259	3.72%	1.446%
6	6.940	821	825	834	rBV	2523325	2453522	9.75%	3.786%
7	7.122	853	856	865	rBV	254044	305346	1.21%	0.471%
8	7.357	892	896	911	rBV	2027427	2006004	7.97%	3.096%
9	7.787	962	969	977	rBV	1357571	1757167	6.98%	2.712%
10	7.987	996	1003	1005	rBV	3580220	4771628	18.96%	7.364%
11	8.069	1013	1017	1025	rVB	1440186	1265604	5.03%	1.953%
12	9.004	1170	1176	1186	rBV	631063	642328	2.55%	0.991%
13	9.145	1192	1200	1203	rBV2	3333271	4032423	16.02%	6.223%
14	9.822	1311	1315	1327	rVB2	1312185	1250997	4.97%	1.931%
15	10.710	1463	1466	1475	rBV	431035	557564	2.22%	0.860%
16	11.157	1540	1542	1545	rBV	421013	329725	1.31%	0.509%
17	11.316	1565	1569	1572	rBV	1204366	1130520	4.49%	1.745%
18	11.586	1612	1615	1618	rBV	454724	339655	1.35%	0.524%
19	11.992	1681	1684	1687	rBV	350980	262150	1.04%	0.405%
20	12.751	1810	1813	1821	rVB2	153417	259468	1.03%	0.400%
21	12.898	1833	1838	1841	rVB	2552620	2357823	9.37%	3.639%
22	13.445	1927	1931	1938	rVB	2267849	2059483	8.18%	3.178%
23	13.774	1984	1987	1994	rVB	314579	371878	1.48%	0.574%
24	13.963	2015	2019	2022	rBV	958940	938658	3.73%	1.449%
25	15.427	2264	2268	2279	rVB	632867	809717	3.22%	1.250%

Sum of corrected areas: 64797285

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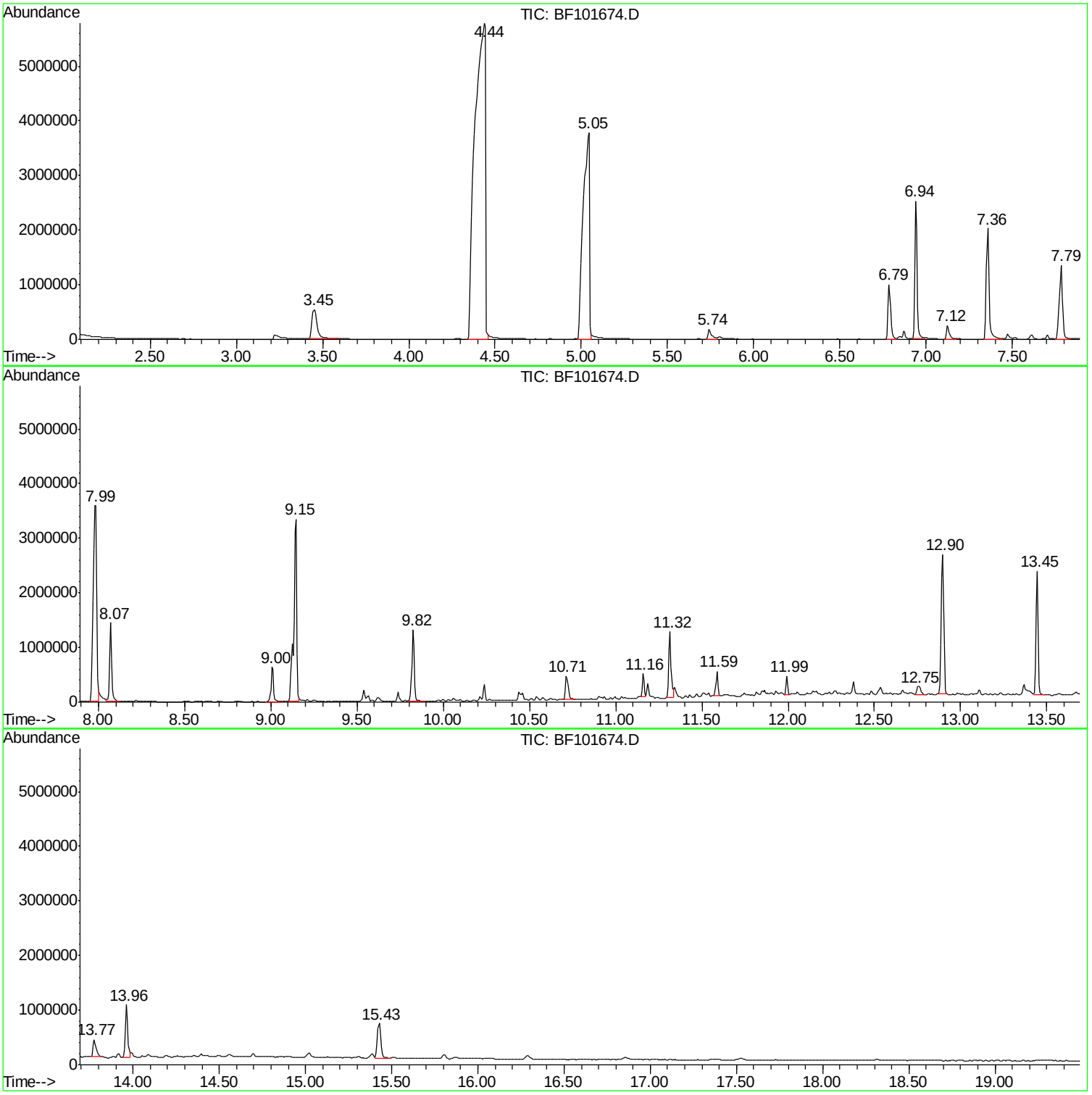
BNA_F
ClientSampleId :
HALSTED-NW

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.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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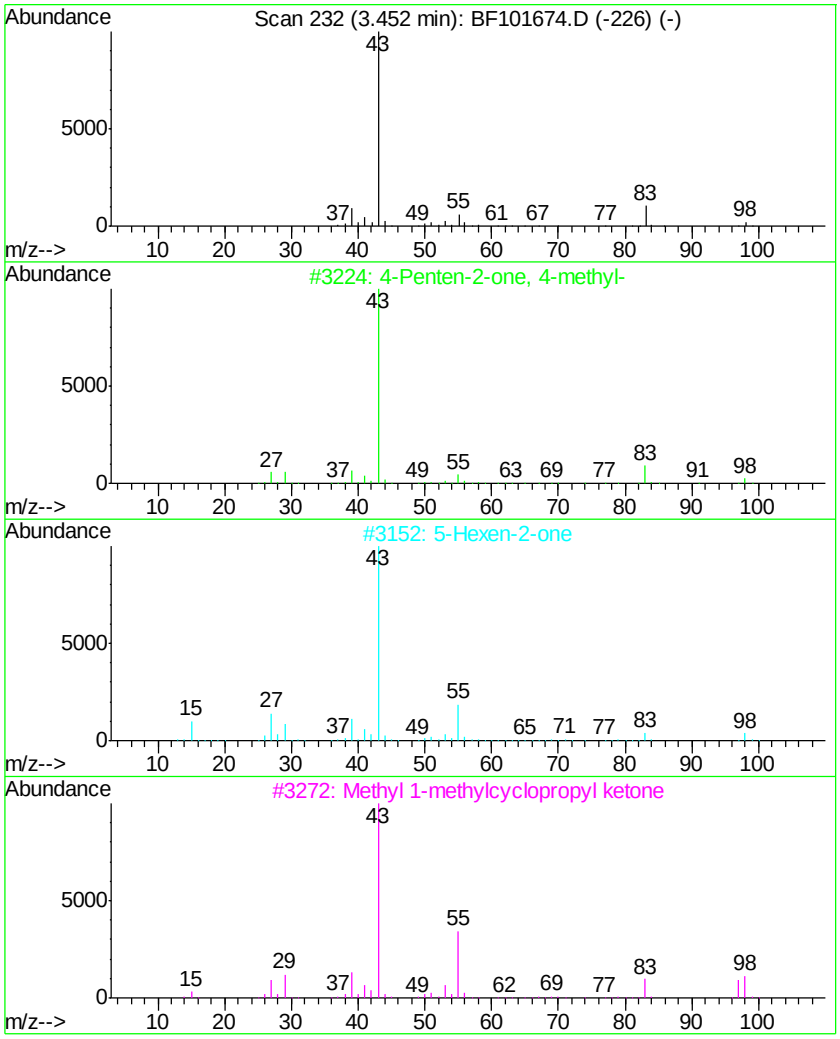
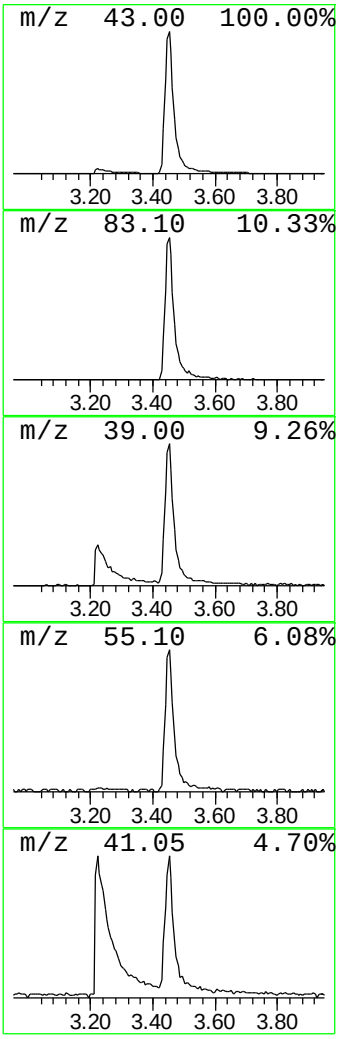
Peak Number 1 4-Penten-2-one, 4-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.45	23.60 ng	1106180	1,4-Dichlorobenzene-d4	6.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	80
2	5-Hexen-2-one	98	C6H10O	000109-49-9	35
3	Methyl 1-methylcyclopropyl ketone	98	C6H10O	001567-75-5	30
4	4-Penten-2-one, 3-methyl-	98	C6H10O	000758-87-2	25
5	4-Hexen-2-one	98	C6H10O	025659-22-7	9





Library Search Compound Report

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Instrument : BNA_F
ClientSampleId : HALSTED-NW

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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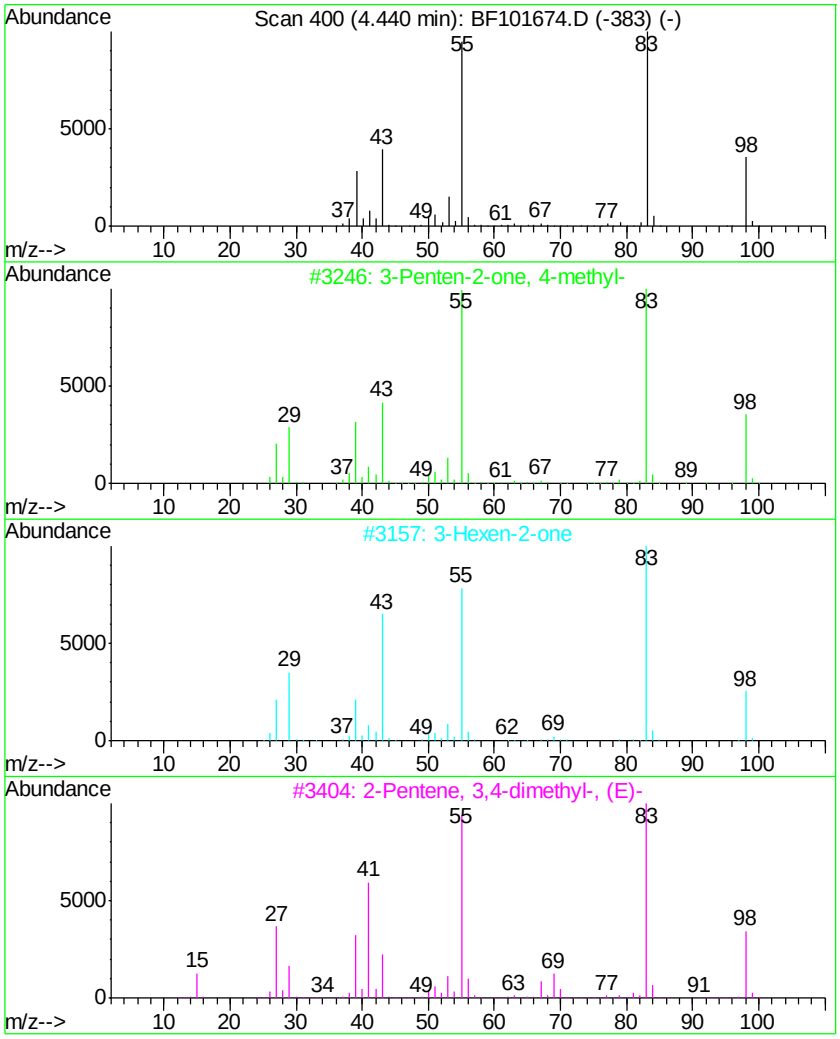
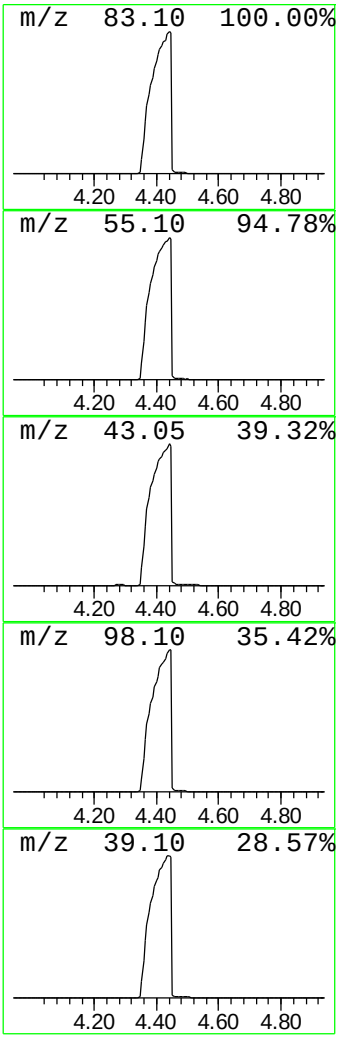
Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.44	537.12 ng	25171200	1,4-Dichlorobenzene-d4	6.79

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, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5	2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	86





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Instrument : BNA_F
ClientSampleId : HALSTED-NW

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
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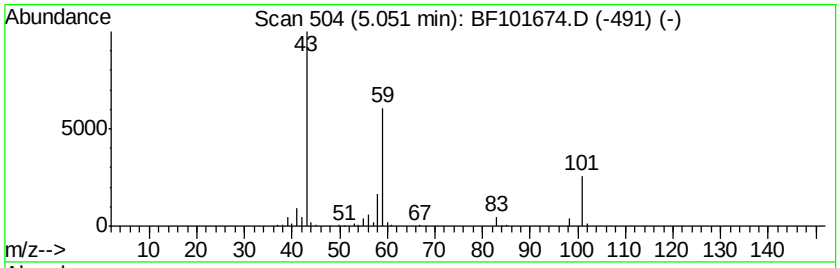
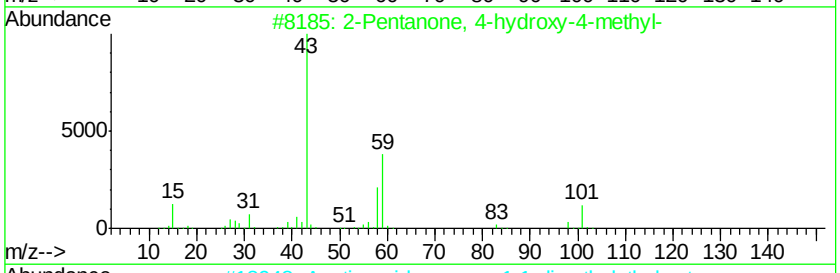
****

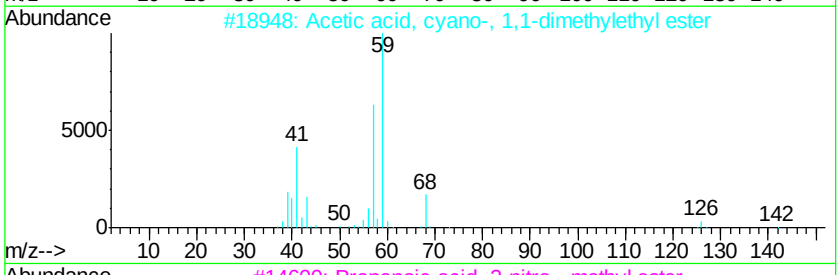
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

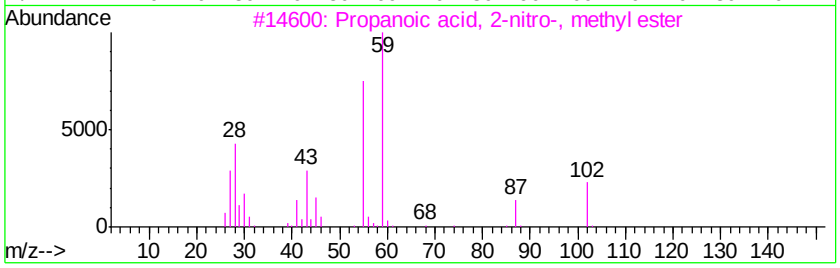
R.T.	EstConc	Area	Relative to ISTD	R.T.
5.05	200.83 ng	9411560	1,4-Dichlorobenzene-d4	6.79

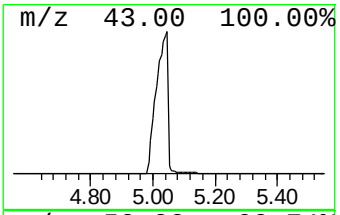
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	Propanoic acid, 2-nitro-, methyl...	133	C4H7NO4	006118-50-9	9
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9
5	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	9

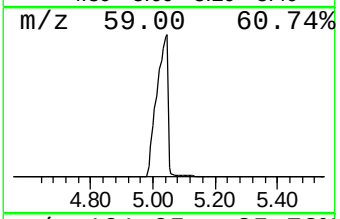


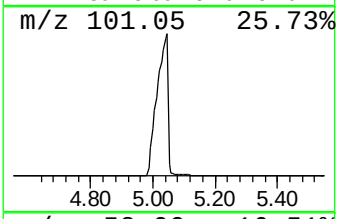


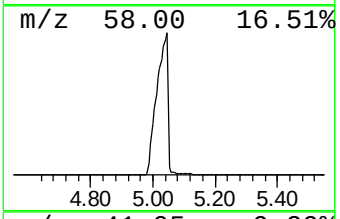


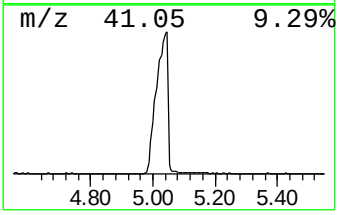












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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
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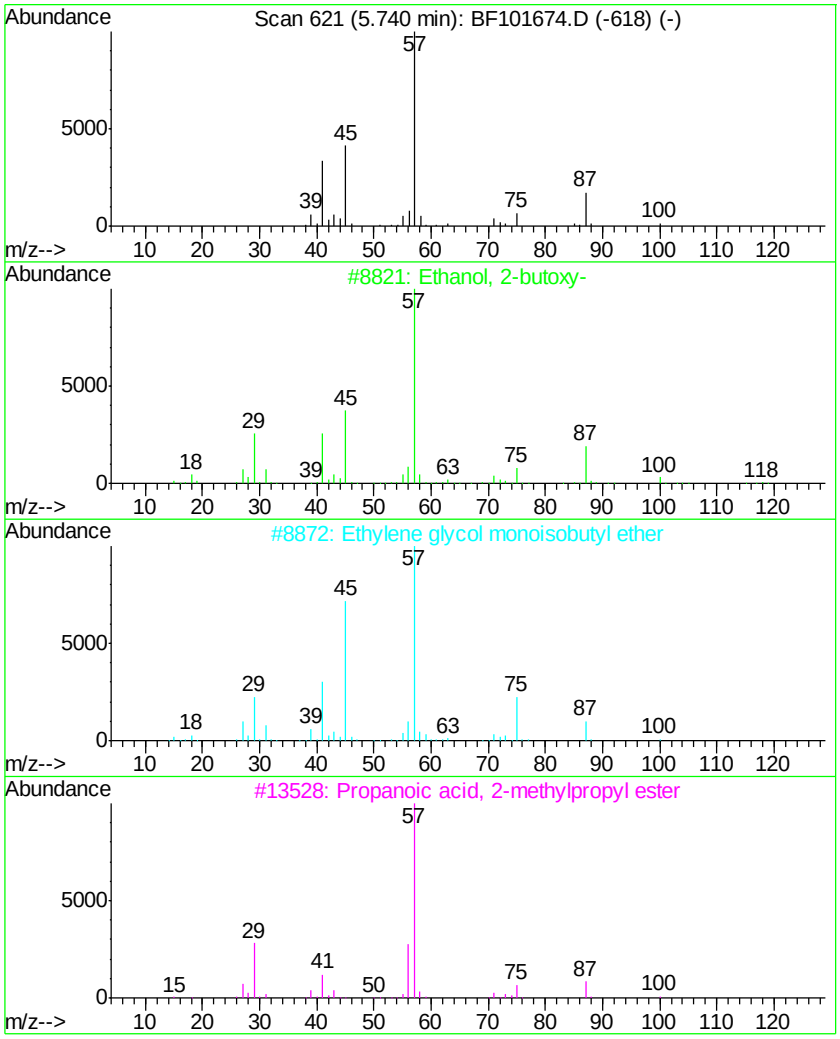
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

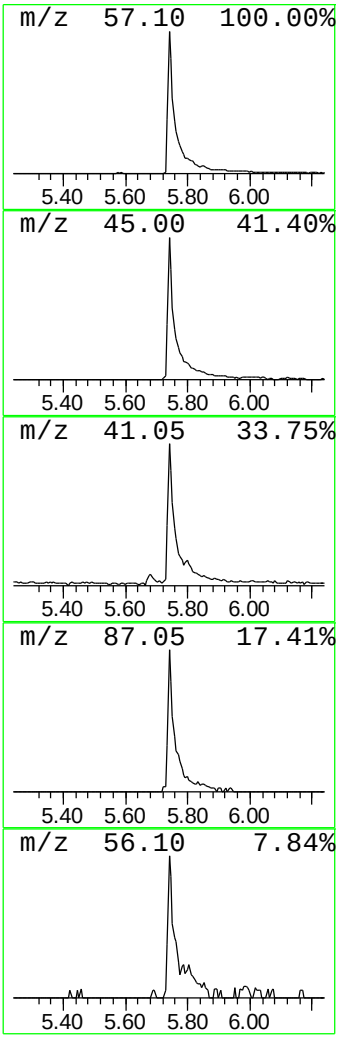
****

Peak Number 4 Ethanol, 2-butoxy- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.74	5.75 ng	269452	1,4-Dichlorobenzene-d4	6.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	78
2	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	45
3	Propanoic acid, 2-methylpropyl e...	130	C7H14O2	000540-42-1	25
4	n-Butyl ether	130	C8H18O	000142-96-1	16
5	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	10





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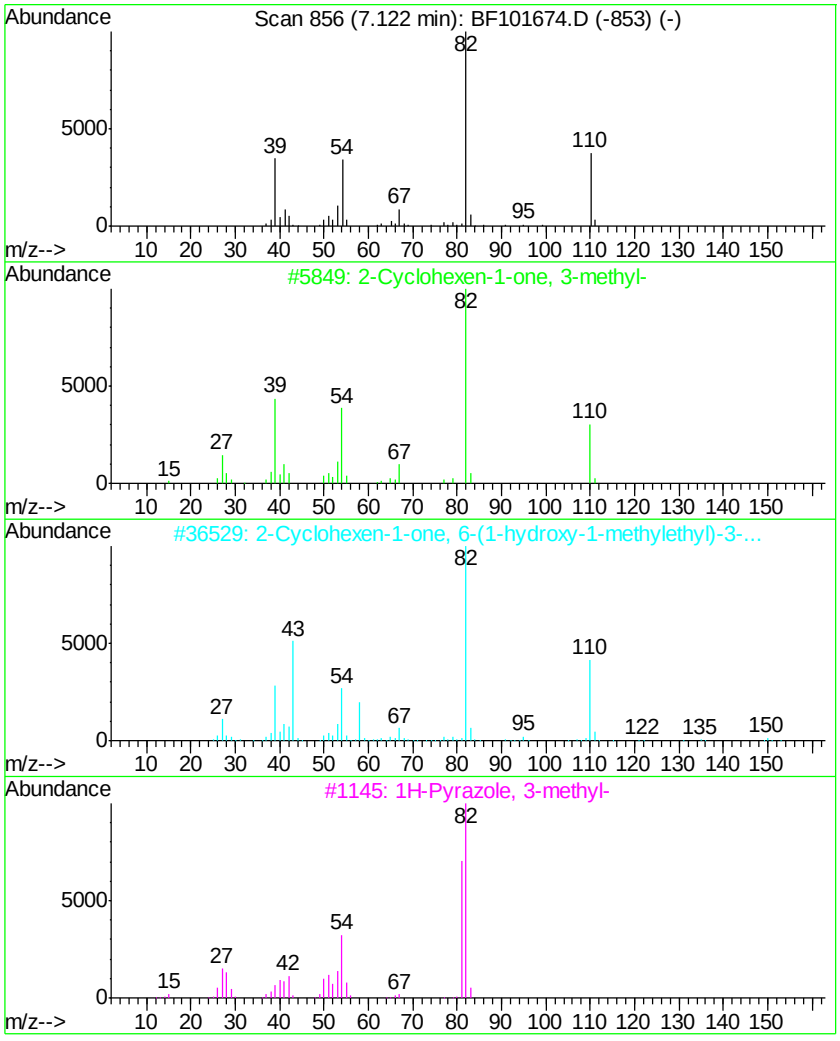
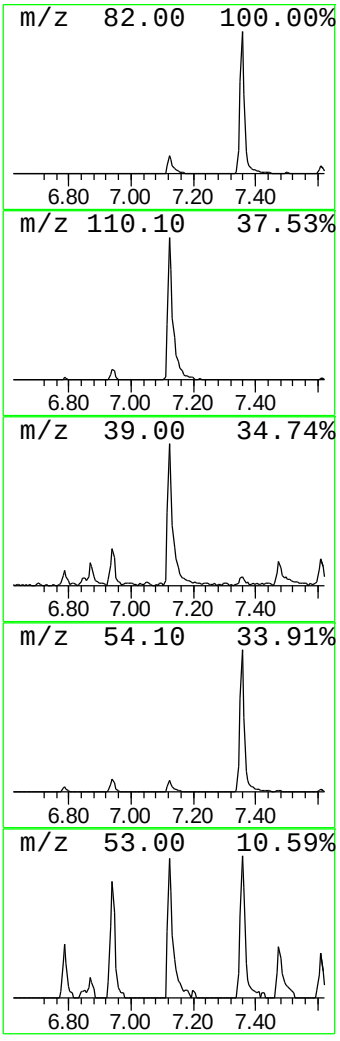
****

Peak Number 6 2-Cyclohexen-1-one, 3-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.12	6.52 ng	305346	1,4-Dichlorobenzene-d4	6.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Cyclohexen-1-one, 3-methyl-	110	C7H10O	001193-18-6	91
2	2-Cyclohexen-1-one, 6-(1-hydroxy...	168	C10H16O2	087791-00-2	78
3	1H-Pyrazole, 3-methyl-	82	C4H6N2	001453-58-3	59
4	1,2,3,6-Tetrahydropyridine	83	C5H9N	000694-05-3	59
5	Betazole	111	C5H9N3	000105-20-4	50





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TIC Library : C:\DATABASE\NIST11.L
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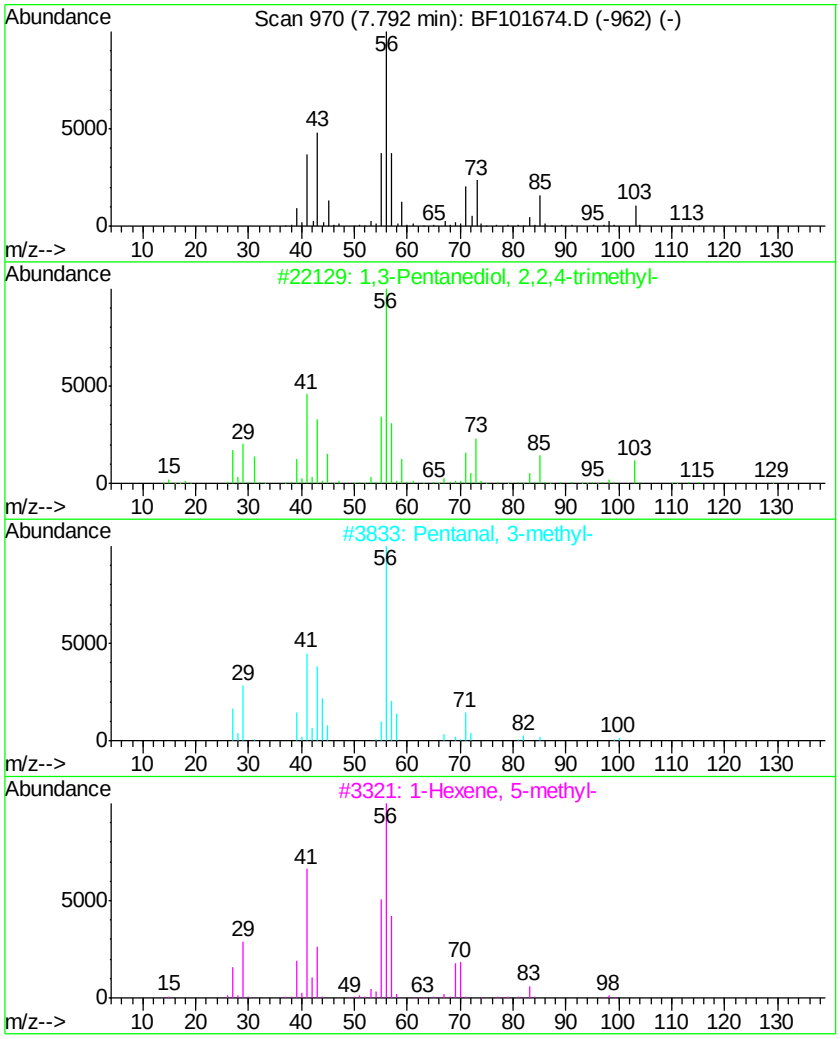
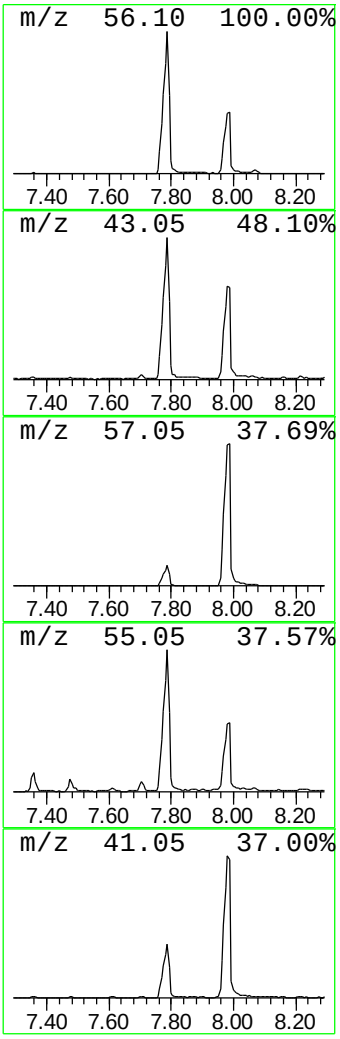
****

Peak Number 7 1,3-Pentanediol, 2,2,4-trim... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.79	27.77 ng	1757170	Naphthalene-d8	8.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Pentanediol, 2,2,4-trimethyl-	146	C8H18O2	000144-19-4	90
2	Pentanal, 3-methyl-	100	C6H12O	015877-57-3	36
3	1-Hexene, 5-methyl-	98	C7H14	003524-73-0	35
4	2,5-Dimethyl-5-hexen-3-ol	128	C8H16O	067760-91-2	34
5	Cyclopentanamine	85	C5H11N	001003-03-8	32





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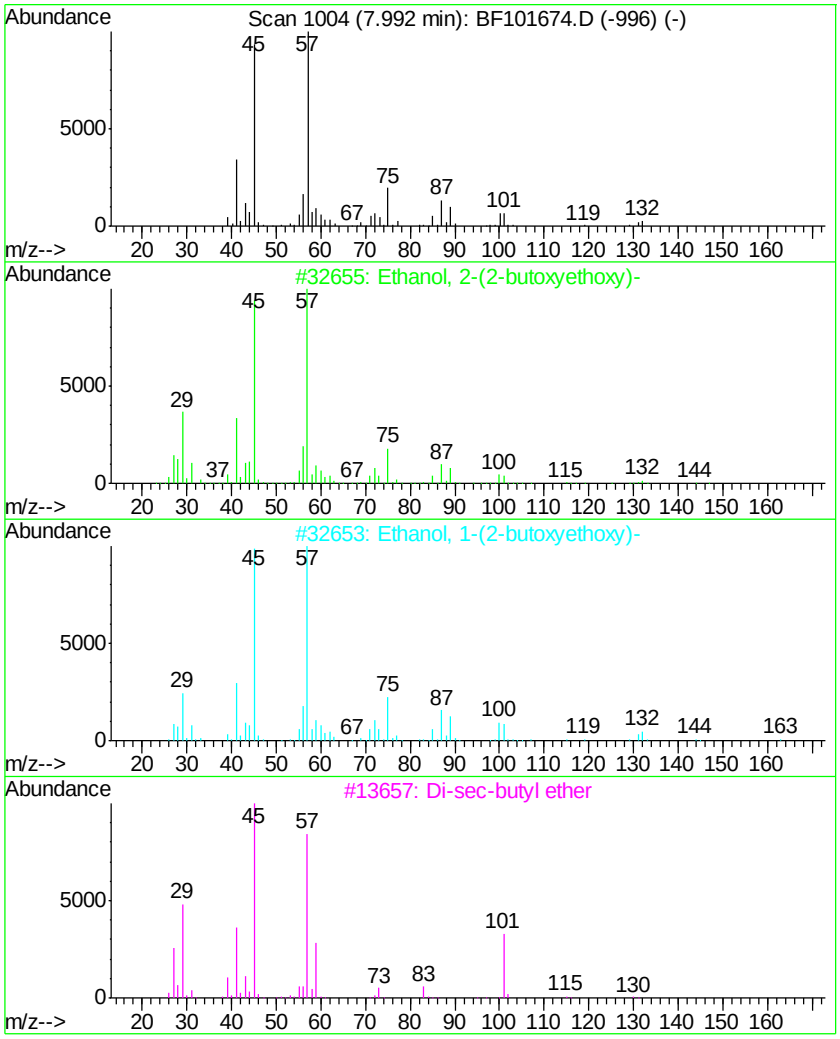
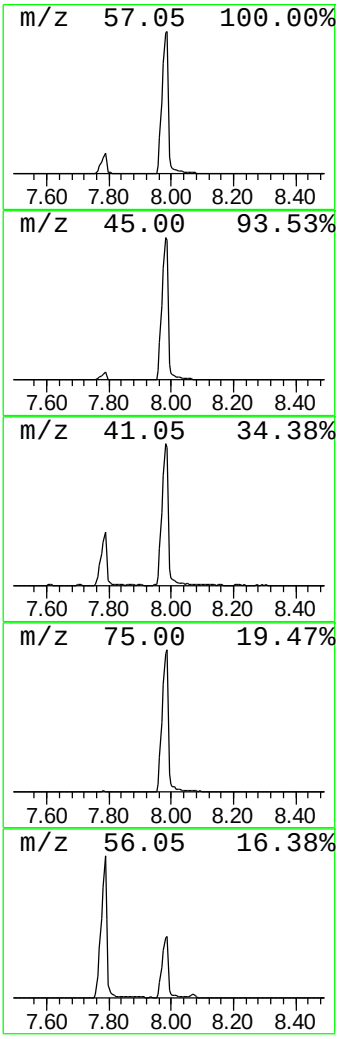
Peak Number 8 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.99	75.40 ng	4771630	Naphthalene-d8	8.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	78
3	Di-sec-butyl ether	130	C8H18O	006863-58-7	53
4	Tetraethylene glycol	194	C8H18O5	000112-60-7	47
5	1-Methoxy-3-methyl-3-butene	100	C6H12O	034752-58-4	47





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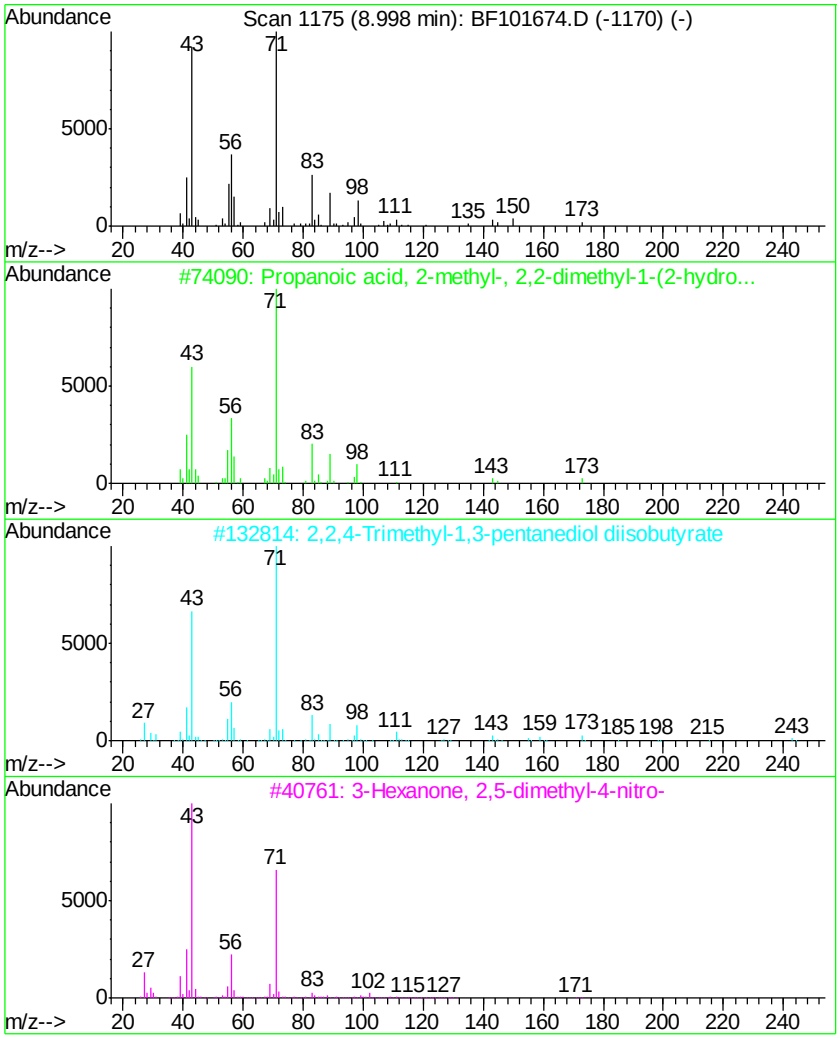
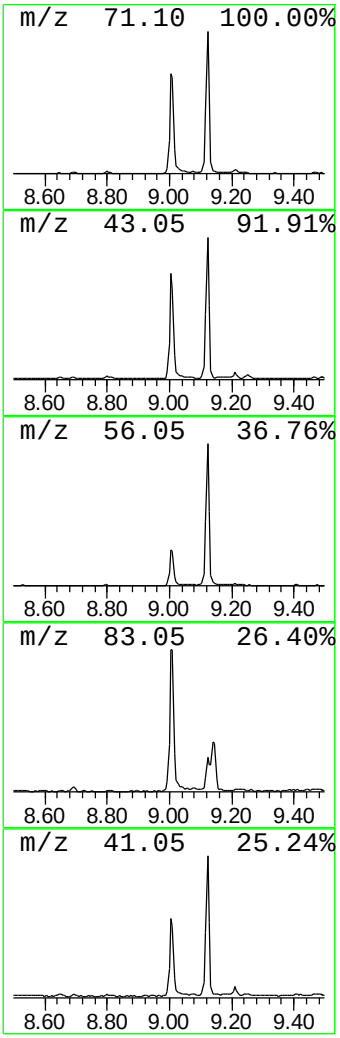
Peak Number 9 Propanoic acid, 2-methyl-, ... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.00	10.27 ng	642328	Acenaphthene-d10	9.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-methyl-, 2,2-d...	216	C12H24O3	074367-33-2	91
2	2,2,4-Trimethyl-1,3-pentanediol ...	286	C16H30O4	006846-50-0	74
3	3-Hexanone, 2,5-dimethyl-4-nitro-	173	C8H15NO3	059906-54-6	47
4	3-Hexenoic acid, 5-hydroxy-2-met...	144	C7H12O3	110678-36-9	45
5	Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	42





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Data File : BF101674.D
Acq On : 23 Dec 2017 00:37
Operator : SJ/JU
Sample : I6957-01
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HALSTED-NW

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.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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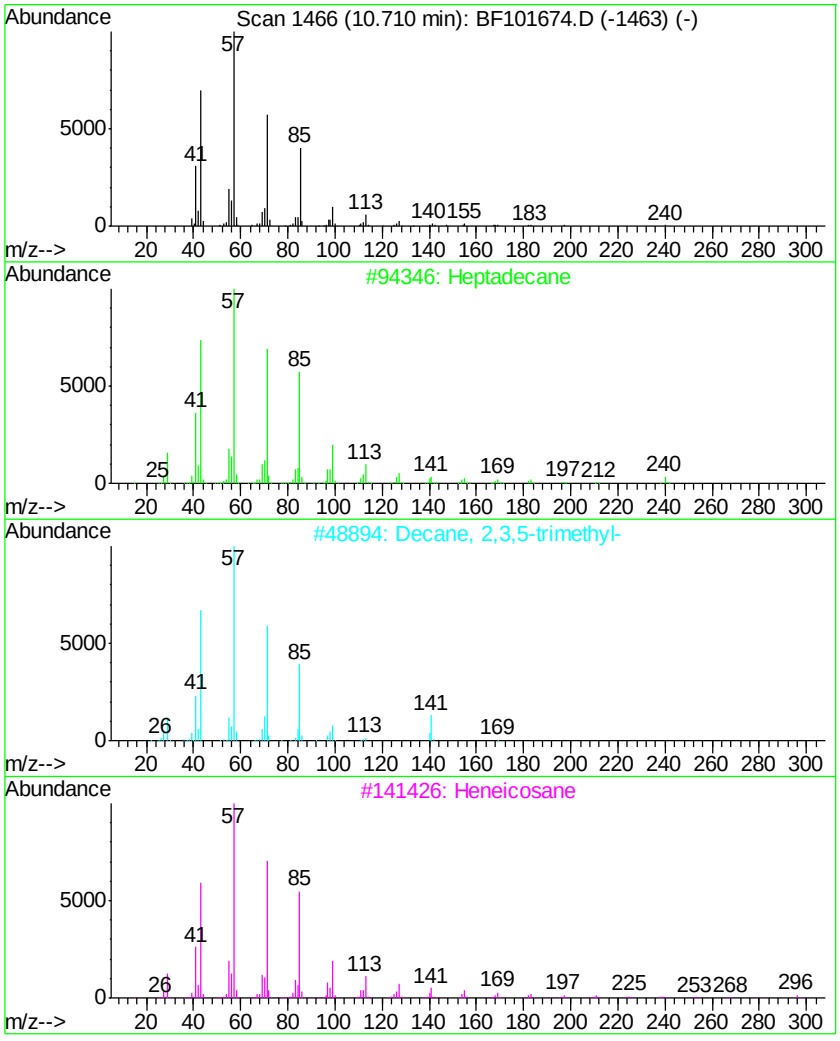
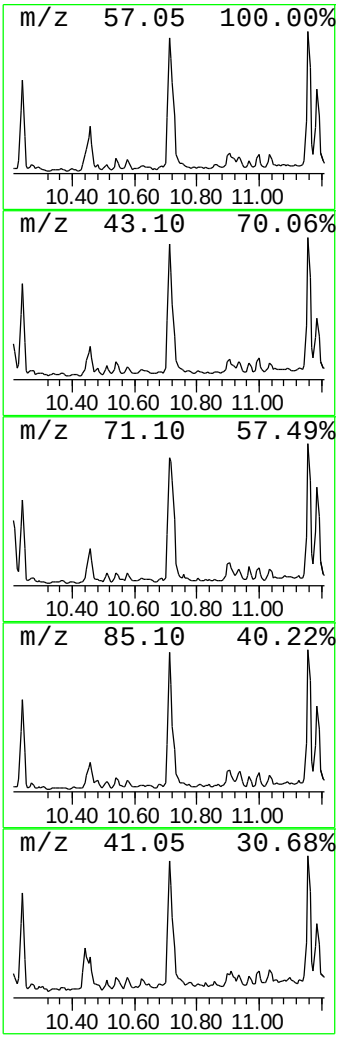
Peak Number 10 Heptadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.71	9.86 ng	557564	Phenanthrene-d10	11.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	97
2	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	86
3	Heneicosane	296	C21H44	000629-94-7	83
4	2-Bromo dodecane	248	C12H25Br	013187-99-0	78
5	Nonane, 5-butyl-	184	C13H28	017312-63-9	72





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ClientSampleId : HALSTED-NW

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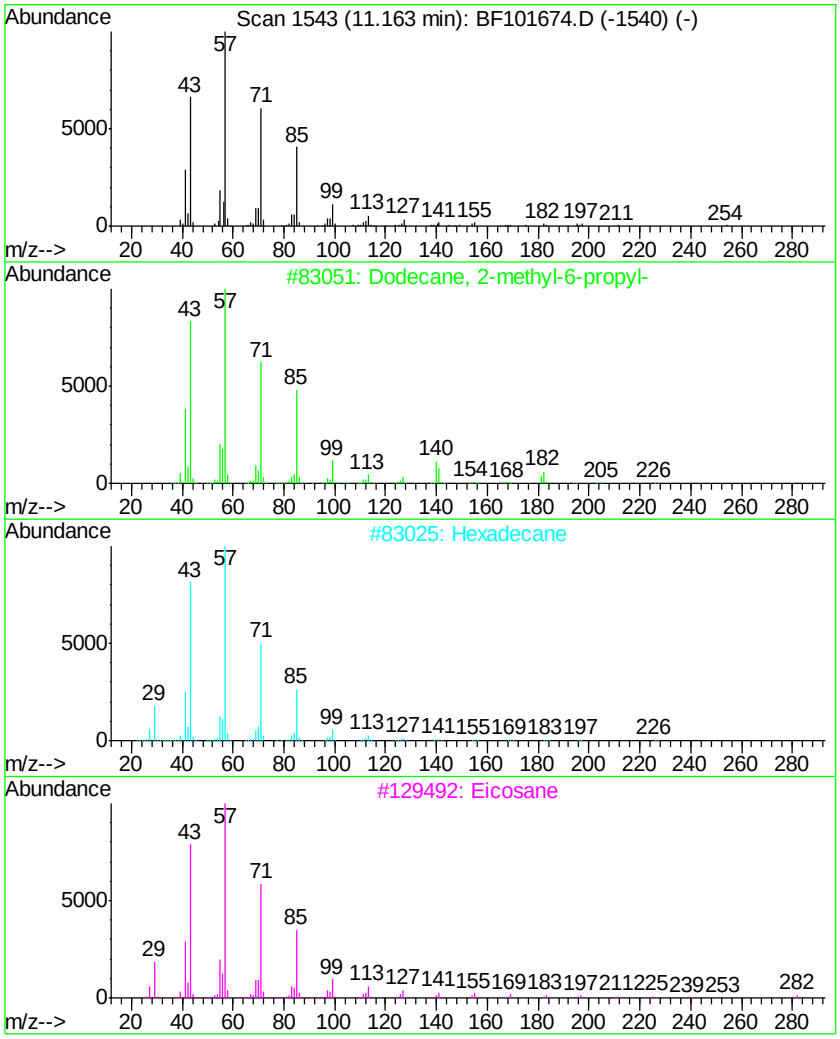
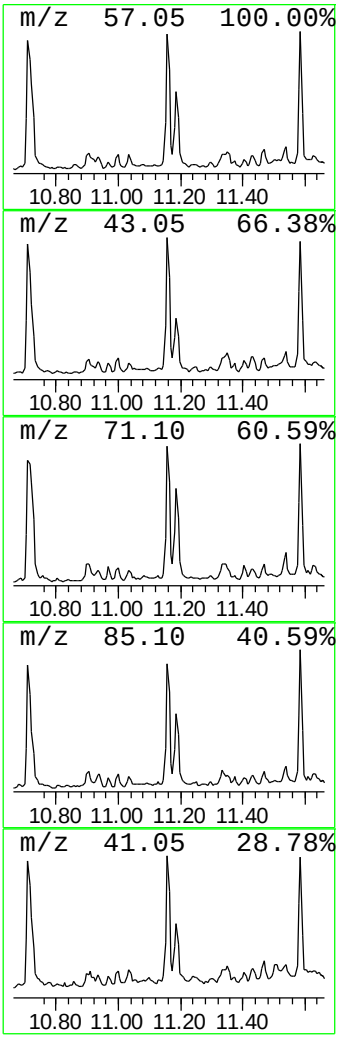
Peak Number 11 Dodecane, 2-methyl-6-propyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.16	5.83 ng	329725	Phenanthrene-d10	11.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	90
2	Hexadecane	226	C16H34	000544-76-3	90
3	Eicosane	282	C20H42	000112-95-8	90
4	Pentadecane	212	C15H32	000629-62-9	90
5	Heptacosane	380	C27H56	000593-49-7	80





Library Search Compound Report

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Data File : BF101674.D
Acq On : 23 Dec 2017 00:37
Operator : SJ/JU
Sample : I6957-01
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HALSTED-NW

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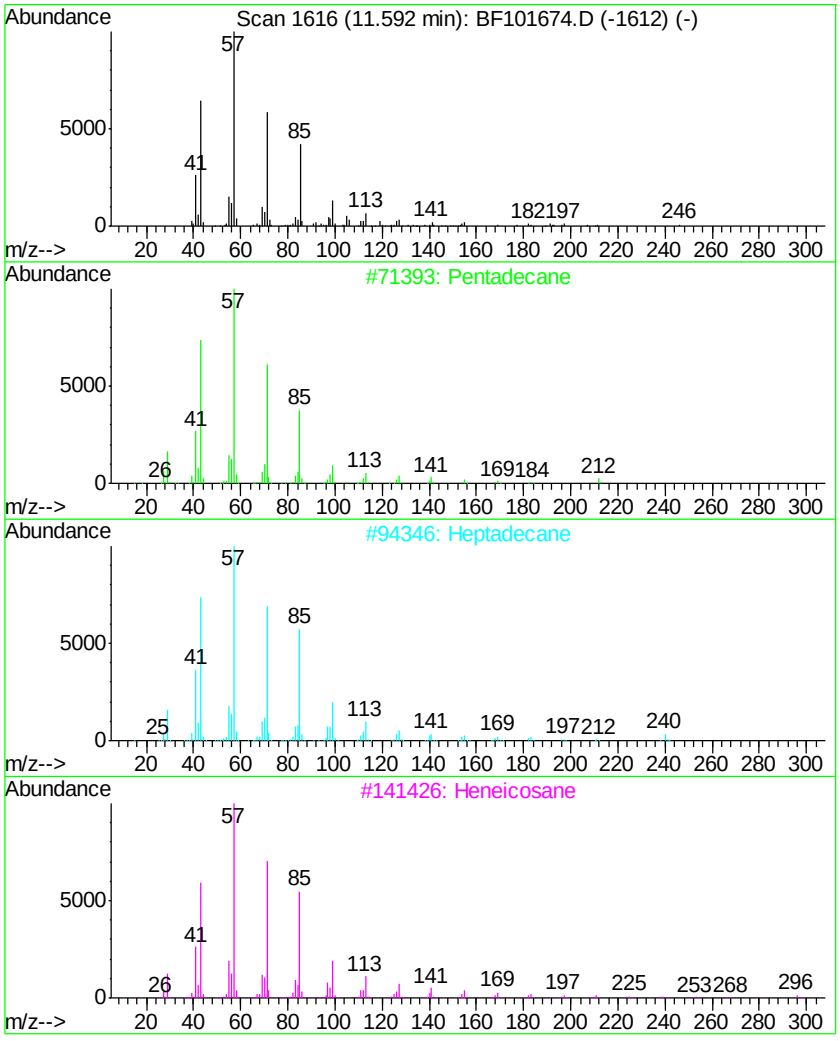
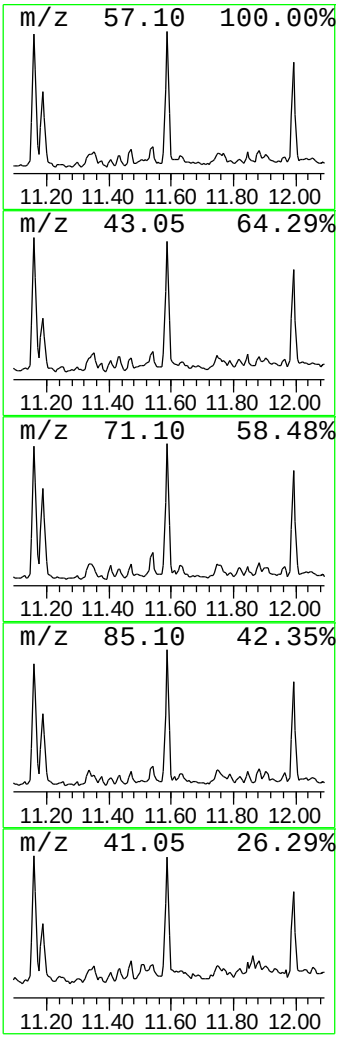
Peak Number 12 Pentadecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.59	6.01 ng	339655	Phenanthrene-d10	11.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane	212	C15H32	000629-62-9	90
2	Heptadecane	240	C17H36	000629-78-7	90
3	Heneicosane	296	C21H44	000629-94-7	90
4	Sulfurous acid, 2-propyl undecyl...	278	C14H30O3S	1000309-12-2	83
5	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	80





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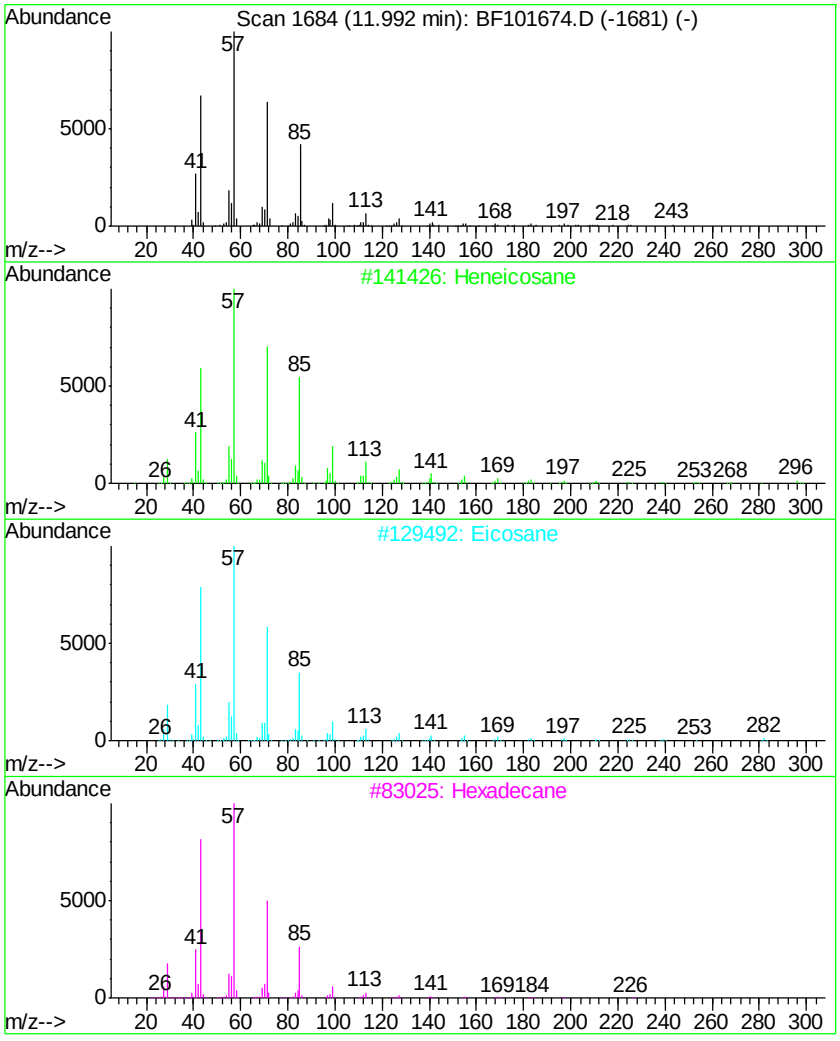
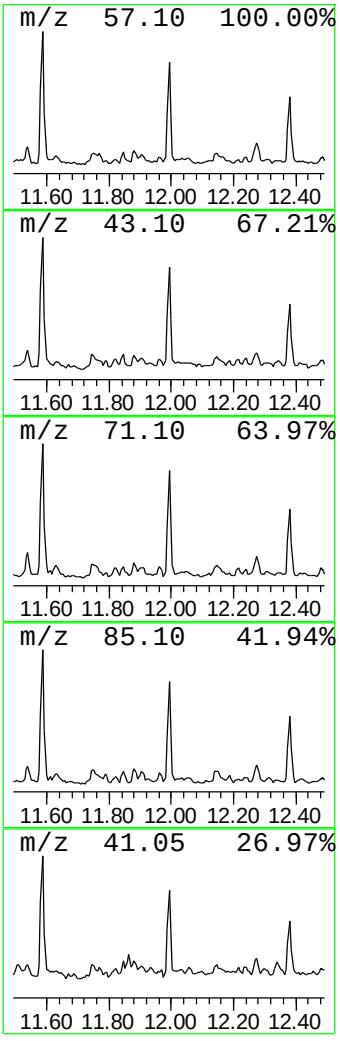
Peak Number 13 Heneicosane Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.99	4.64 ng	262150	Phenanthrene-d10	11.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	90
2	Eicosane	282	C20H42	000112-95-8	90
3	Hexadecane	226	C16H34	000544-76-3	90
4	Nonadecane	268	C19H40	000629-92-5	87
5	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	86





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ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HALSTED-NW

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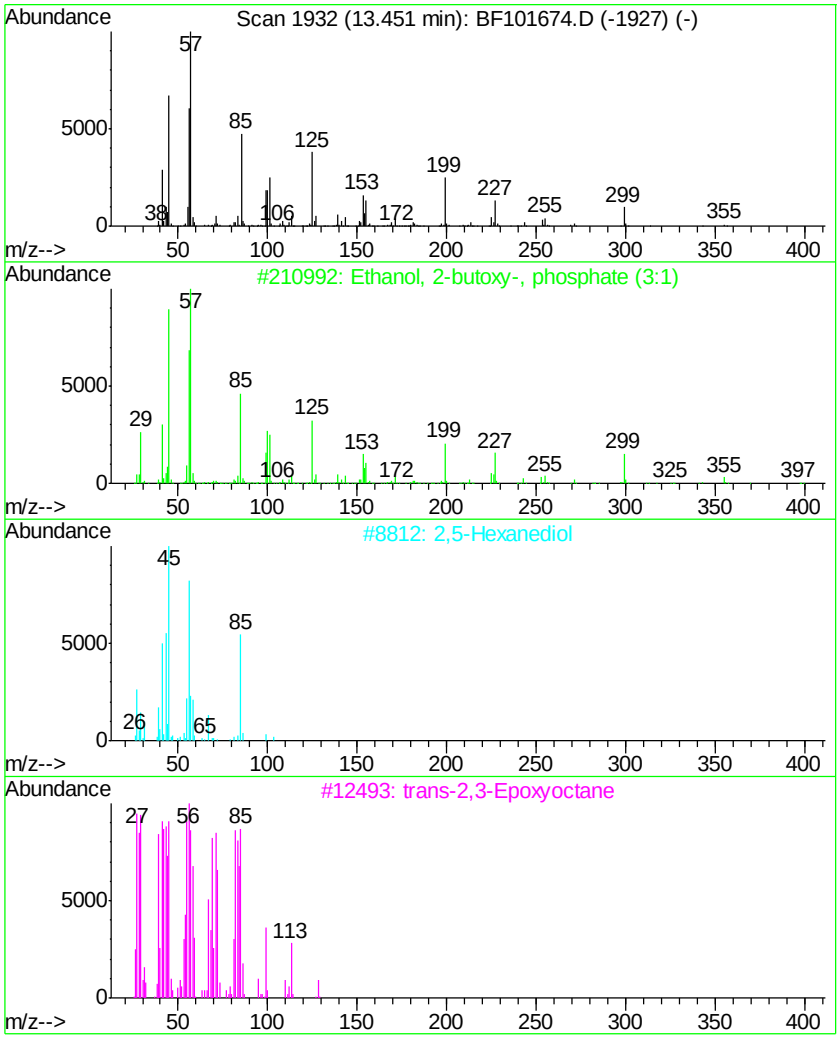
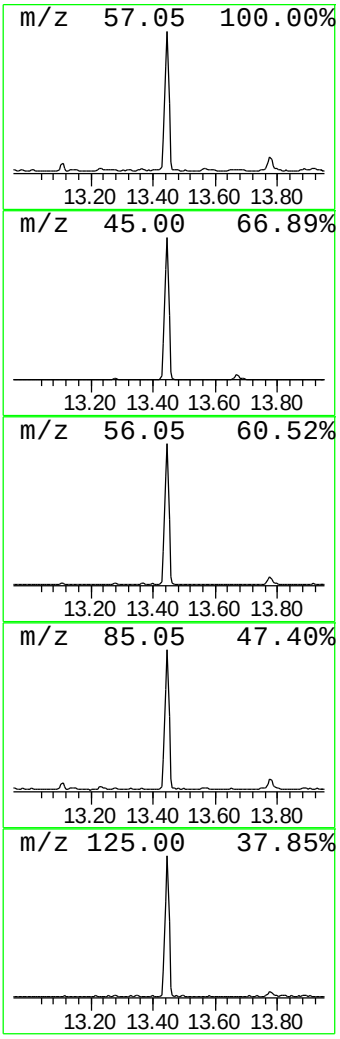
Peak Number 14 Ethanol, 2-butoxy-, phospha... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.45	43.88 ng	2059480	Chrysene-d12	13.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-butoxy-, phosphate (3:1)	398	C18H39O7P	000078-51-3	86
2	2,5-Hexanediol	118	C6H14O2	002935-44-6	43
3	trans-2,3-Epoxyoctane	128	C8H16O	028180-70-3	37
4	Butane, 1,1'-[oxybis(2,1-ethaned...	218	C12H26O3	000112-73-2	35
5	2-Propanone, ethylhydrazone	100	C5H12N2	007422-99-3	25





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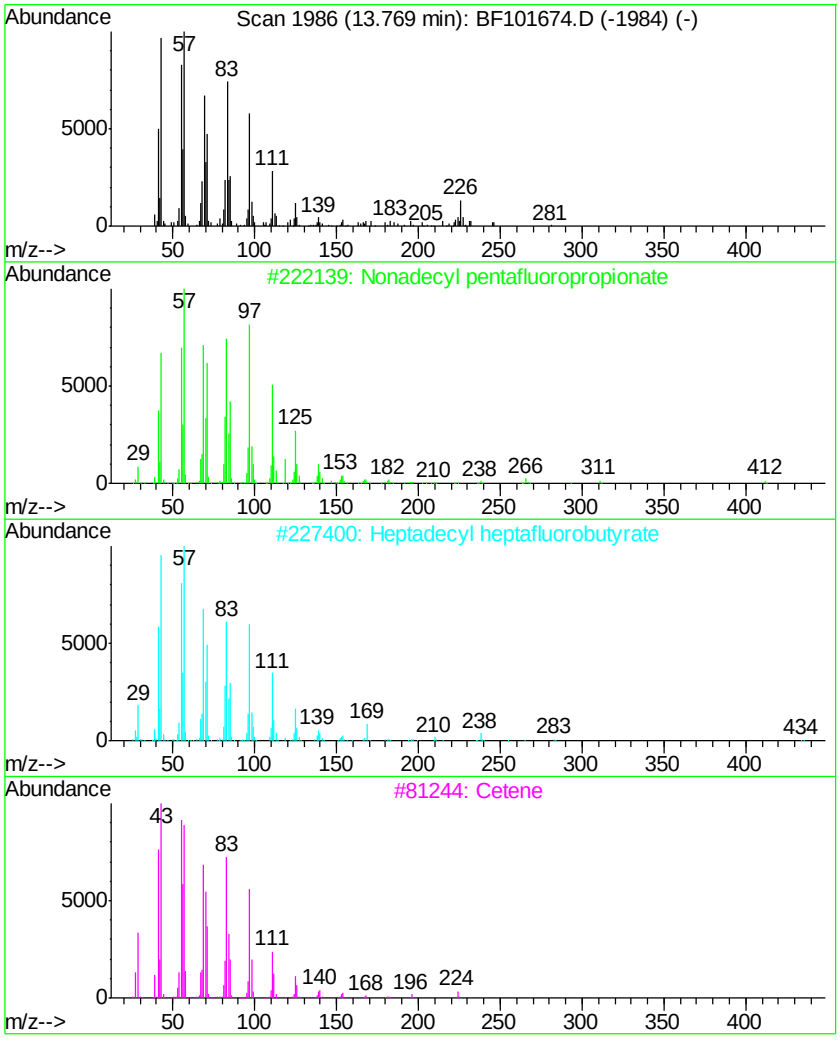
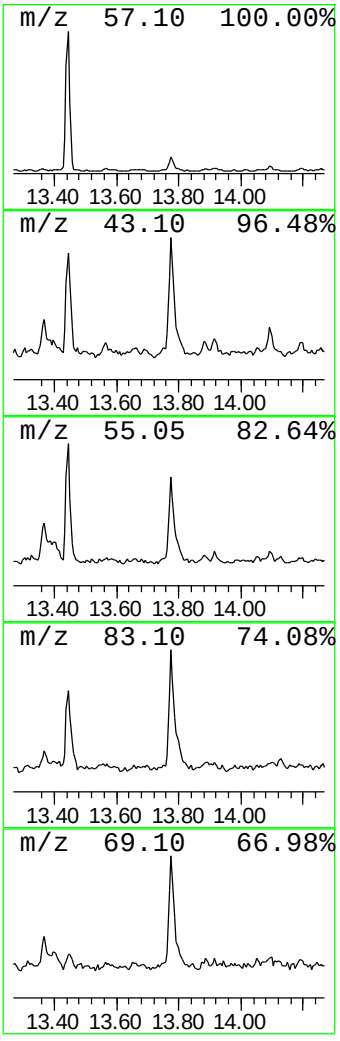
Peak Number 15 Nonadecyl pentafluoropropio... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.77	7.92 ng	371878	Chrysene-d12	13.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
3	Cetene	224	C16H32	000629-73-2	91
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
5	Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	91





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
4-Penten-2-one, 4...	3.45	23.6	ng	1106180	1	6.79	937259	20.0
3-Penten-2-one, 4...	4.44	537.1	ng	25171200	1	6.79	937259	20.0
2-Pentanone, 4-hy...	5.05	200.8	ng	9411560	1	6.79	937259	20.0
Ethanol, 2-butoxy-	5.74	5.8	ng	269452	1	6.79	937259	20.0
2-Cyclohexen-1-on...	7.12	6.5	ng	305346	1	6.79	937259	20.0
1,3-Pentanediol, ...	7.79	27.8	ng	1757170	2	8.07	1265600	20.0
Ethanol, 2-(2-but...	7.99	75.4	ng	4771630	2	8.07	1265600	20.0
Propanoic acid, 2...	9.00	10.3	ng	642328	3	9.82	1251000	20.0
Heptadecane	10.71	9.9	ng	557564	4	11.32	1130520	20.0
Dodecane, 2-methy...	11.16	5.8	ng	329725	4	11.32	1130520	20.0
Pentadecane	11.59	6.0	ng	339655	4	11.32	1130520	20.0
Heneicosane	11.99	4.6	ng	262150	4	11.32	1130520	20.0
Ethanol, 2-butoxy...	13.45	43.9	ng	2059480	5	13.96	938658	20.0
Nonadecyl pentafl...	13.77	7.9	ng	371878	5	13.96	938658	20.0