LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121218\
Data File : BF111329.D
Acq On : 12 Dec 2018 18:48
Operator : JU/SJ
Sample : J6241-55
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TW-2

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121218.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	4.987	485	493	500	rBV2	218677	307746	3.07%	0.508%
2	5.404	560	564	573	rBV	3445464	3157428	31.52%	5.207%
3	6.416	732	736	745	rBV2	2390703	2502700	24.99%	4.127%
4	6.557	756	760	764	rBV	5576204	5512334	55.04%	9.091%
5	6.793	796	800	803	rBV	2224781	1966593	19.64%	3.243%
6	6.951	822	827	830	rBV	7970579	7266194	72.55%	11.983%
7	7.357	889	896	899	rBV	5591134	6254786	62.45%	10.315%
8	7.569	929	932	935	rBV	169077	146078	1.46%	0.241%
9	7.975	998	1001	1008	rBV	368354	390747	3.90%	0.644%
10	8.075	1014	1018	1021	rBV	3075191	2620029	26.16%	4.321%
11	9.157	1196	1202	1205	rBV	9870409	10015654	100.00%	16.518%
12	9.245	1212	1217	1220	rBV3	78986	116820	1.17%	0.193%
13	9.539	1264	1267	1270	rBV	529790	414118	4.13%	0.683%
14	9.828	1310	1316	1320	rBV	3051834	2710473	27.06%	4.470%
15	10.110	1359	1364	1367	rBV	92932	126778	1.27%	0.209%
16	10.610	1445	1449	1453	rBV	3167927	3002752	29.98%	4.952%
17	10.739	1469	1471	1476	rBV3	77108	111685	1.12%	0.184%
18	10.980	1509	1512	1516	rVB4	123512	123312	1.23%	0.203%
19	11.057	1523	1525	1533	rVB5	98583	152667	1.52%	0.252%
20	11.310	1564	1568	1571	rBV	2316419	1912563	19.10%	3.154%
21	11.845	1656	1659	1668	rBV	1285283	1303976	13.02%	2.151%
22	12.633	1789	1793	1802	rBV	1615032	1629418	16.27%	2.687%
23	12.898	1834	1838	1841	rBV	5926910	5503552	54.95%	9.077%
24	13.804	1989	1992	2000	rVB	576380	717502	7.16%	1.183%
25	13.945	2012	2016	2024	rVB	1716039	1568811	15.66%	2.587%
26	15.380	2256	2260	2265	rVB	943025	1100423	10.99%	1.815%

Sum of corrected areas: 60635139

LSC Report - Integrated Chromatogram

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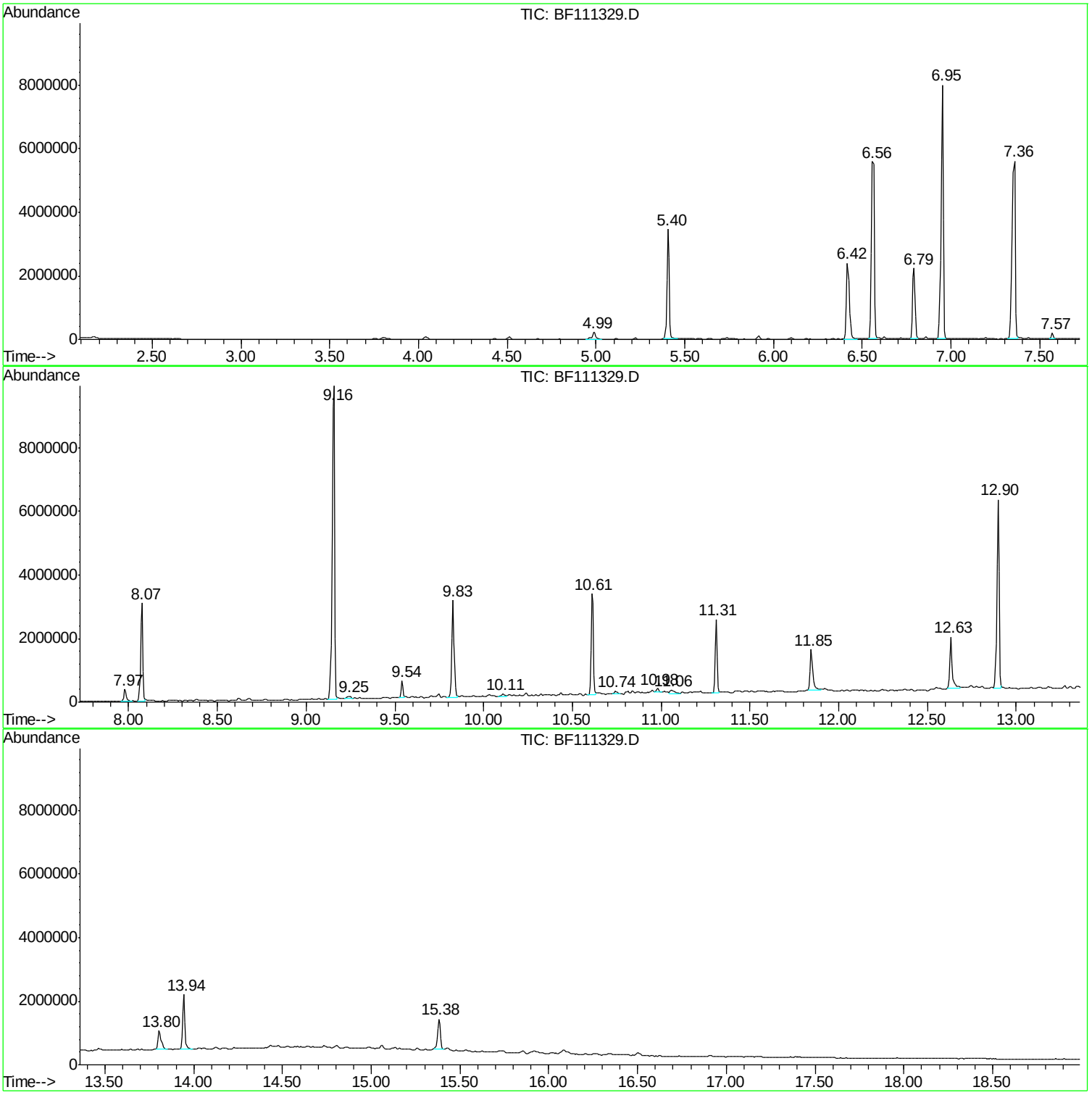
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TW-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121218.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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Instrument : BNA_F
ClientSampleId : TW-2

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

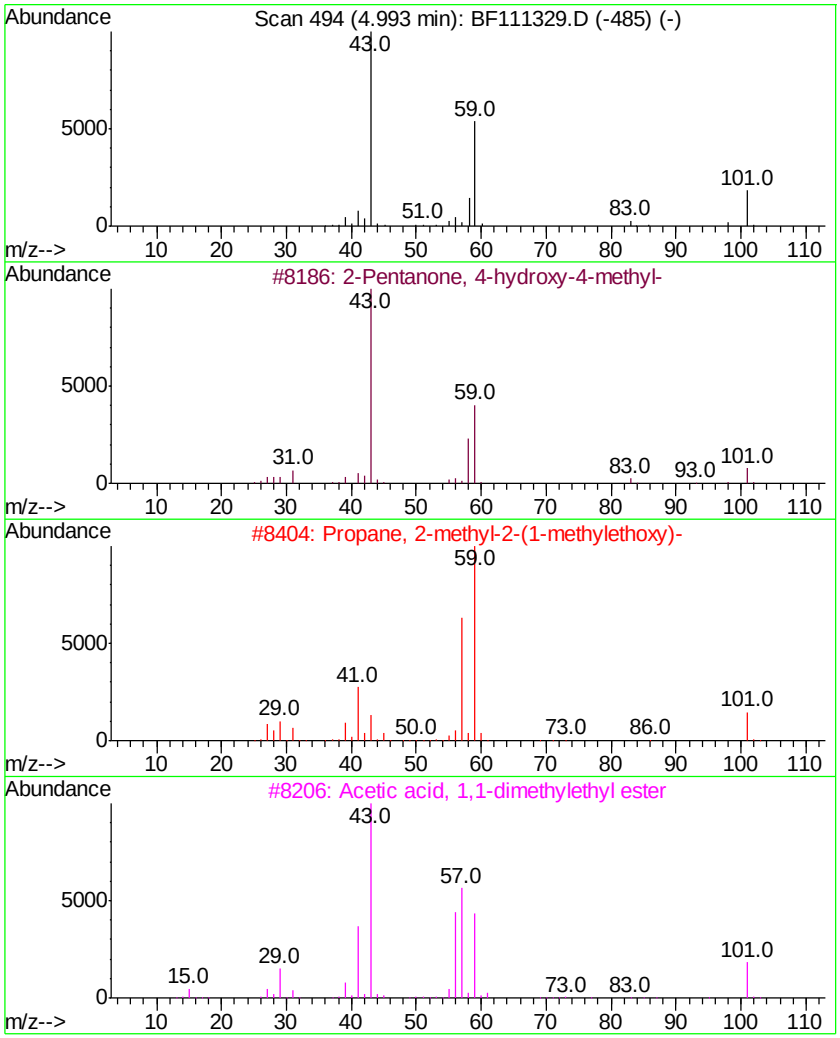
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

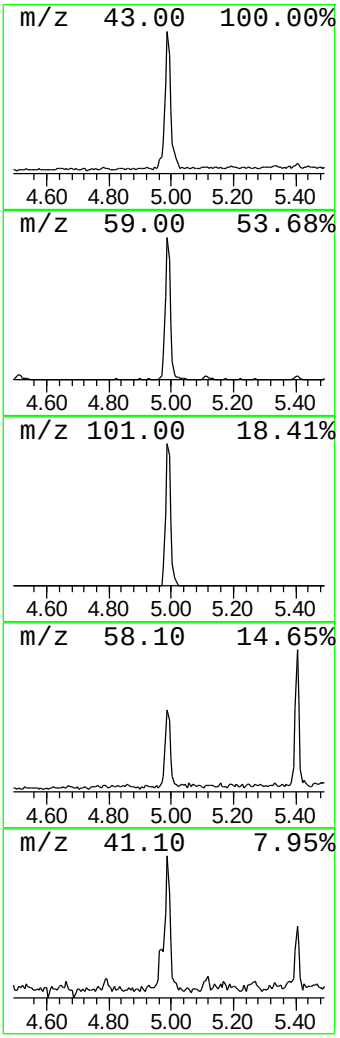
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.99	3.13 ng	307746	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	45
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23





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Operator : JU/SJ
Sample : J6241-55
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TW-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121218.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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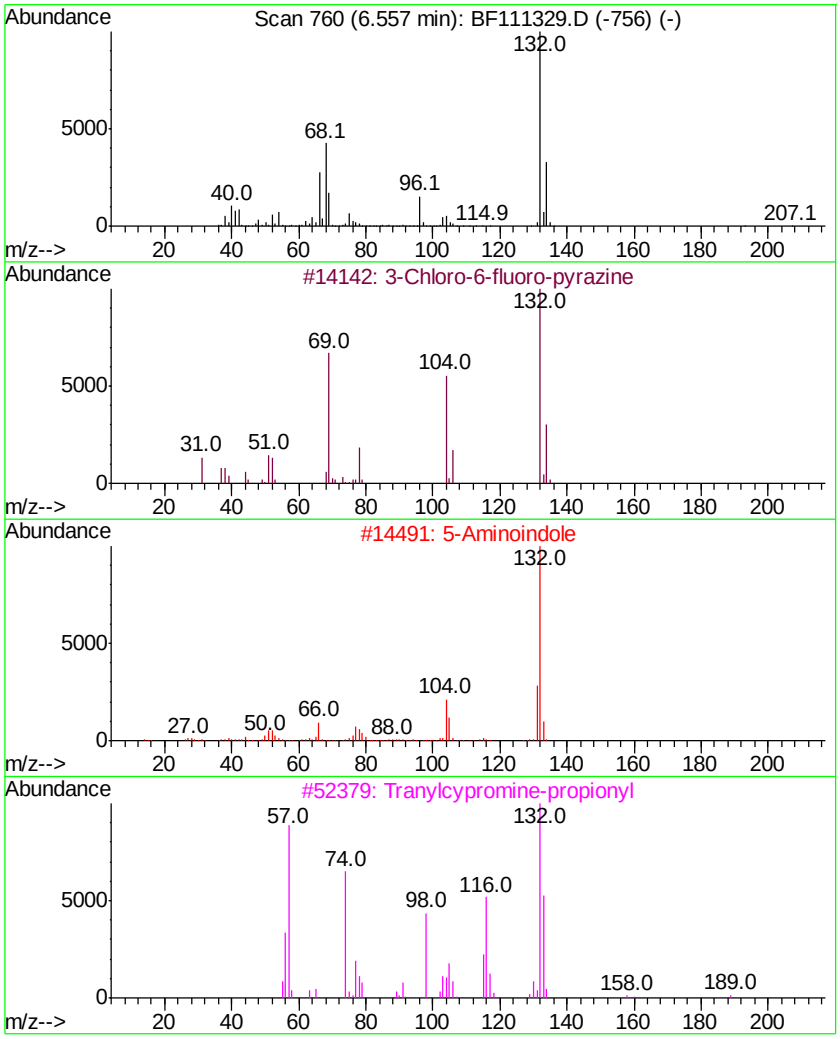
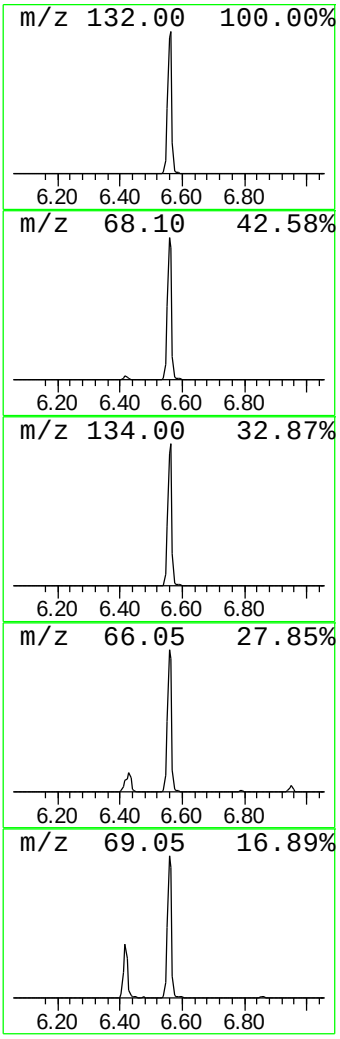
Peak Number 2 unknown6.56 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	56.06 ng	5512330	1,4-Dichlorobenzene-d4	6.79

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	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





Library Search Compound Report

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Sample : J6241-55
Misc :
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Instrument : BNA_F
ClientSampleId : TW-2

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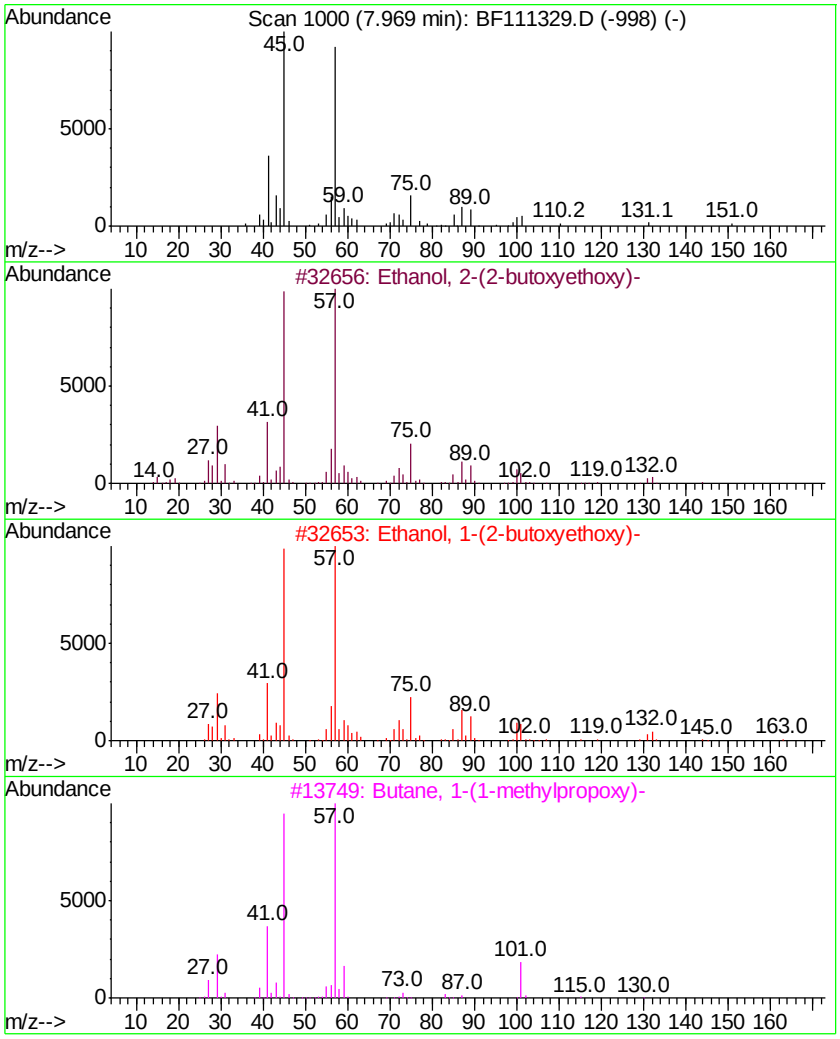
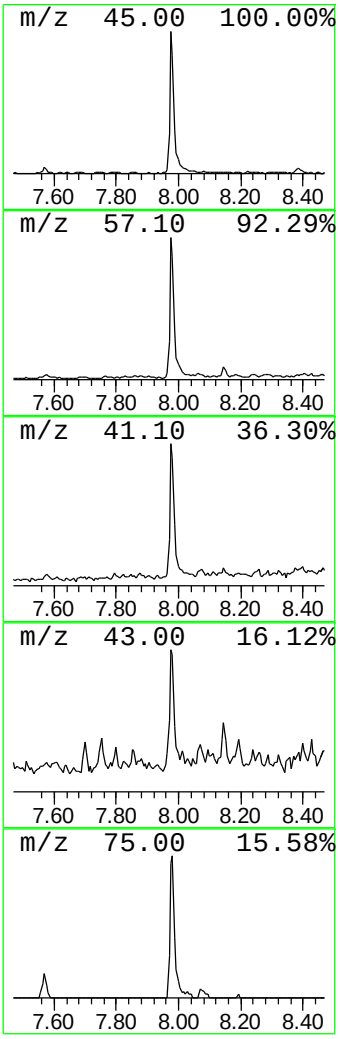
Peak Number 4 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.97	2.98 ng	390747	Naphthalene-d8	8.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	83
2	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3	Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	53
4	Sulfurous acid, bis(1-methylprop...	194	C8H18O3S	024769-51-5	53
5	Heptaethylene glycol	326	C14H30O8	005617-32-3	50





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ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TW-2

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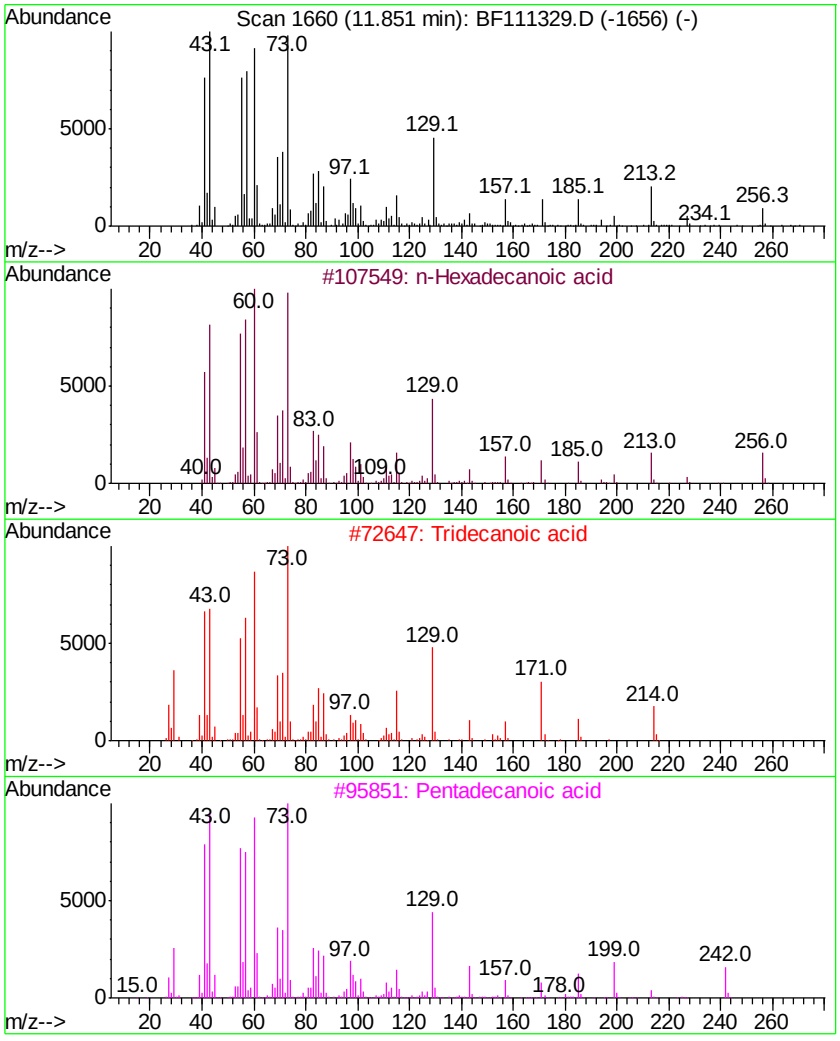
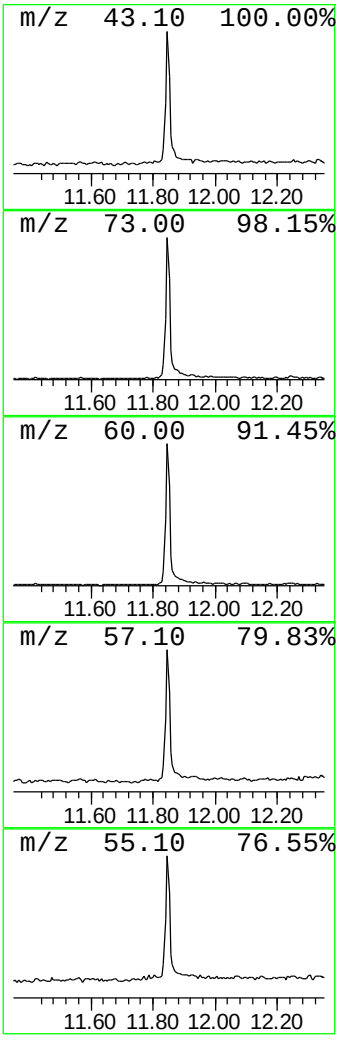
Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.85	13.64 ng	1303980	Phenanthrene-d10	11.31

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	78
5	n-Decanoic acid	172	C10H20O2	000334-48-5	64





Library Search Compound Report

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Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TW-2

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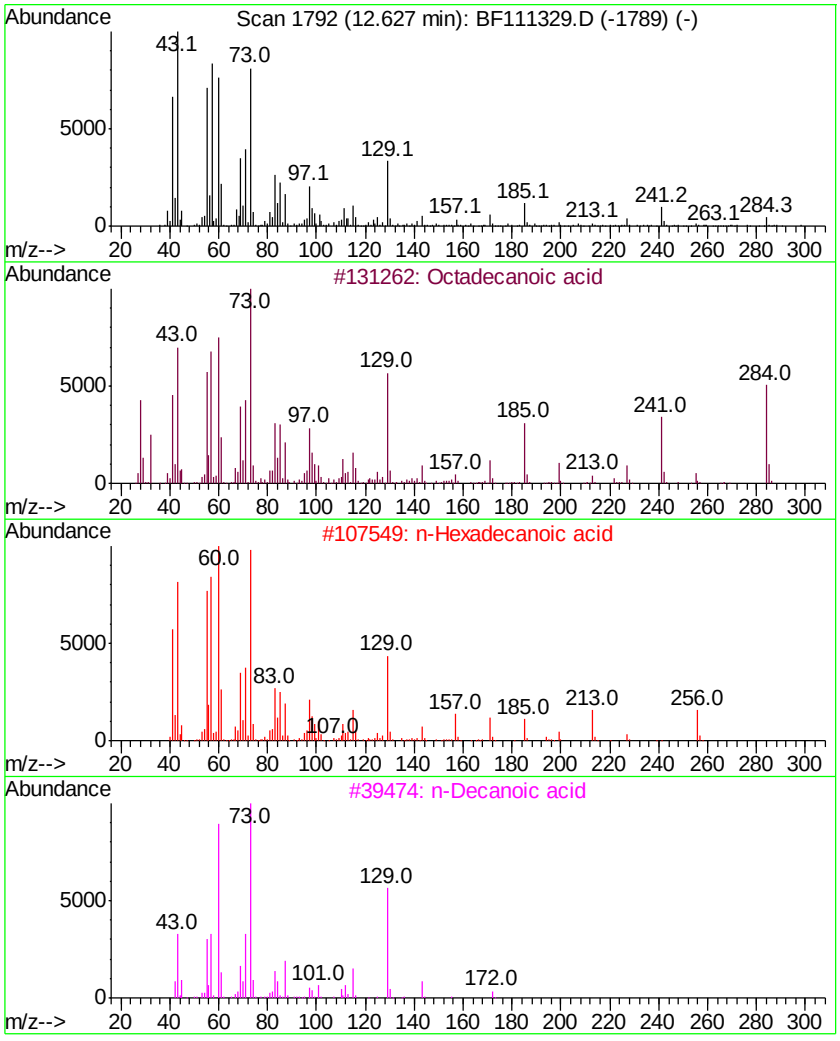
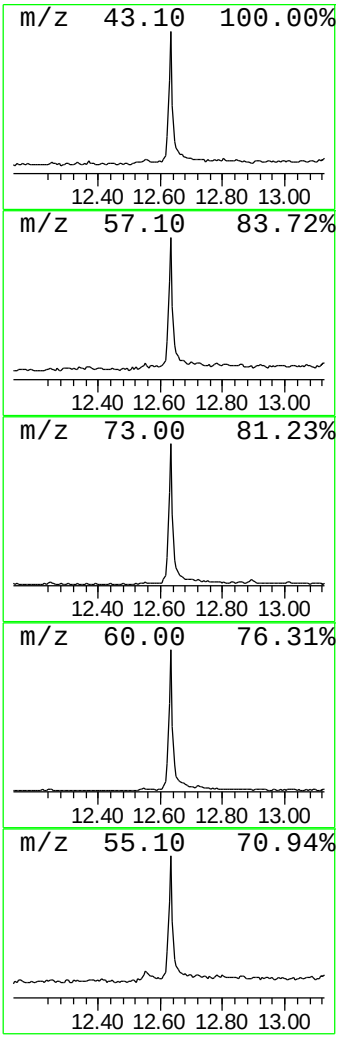
****

Peak Number 6 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.63	20.77 ng	1629420	Chrysene-d12	13.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
3	n-Decanoic acid	172	C10H20O2	000334-48-5	91
4	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	87
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	80





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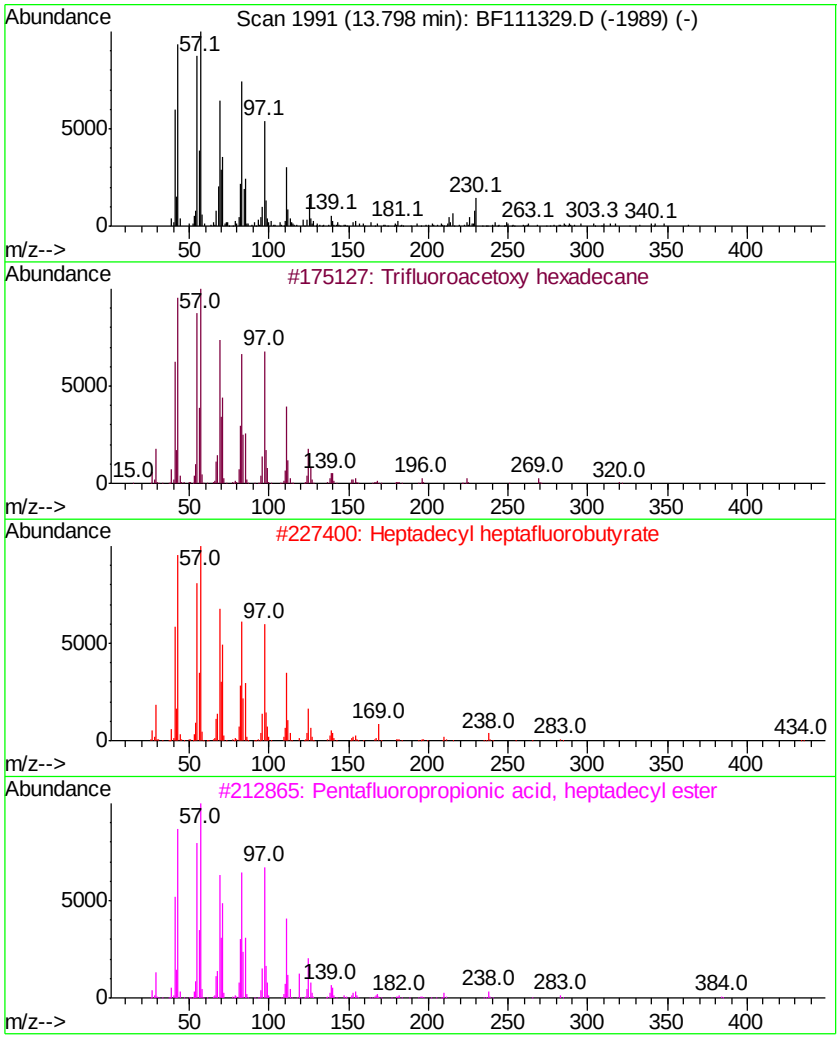
TIC Integration Parameters: LSCINT.P

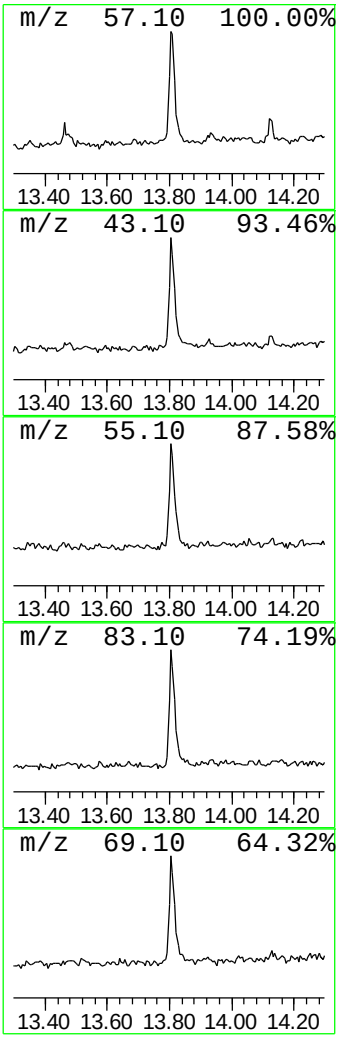
****

Peak Number 7 Trifluoroacetoxy hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.80	9.15 ng	717502	Chrysene-d12	13.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
3	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91
4	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	91
5	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91





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...	4.99	3.1	ng	307746	1	6.79	1966590	20.0
unknown6.56	6.56	56.1	ng	5512330	1	6.79	1966590	20.0
Ethanol, 2-(2-but...	7.97	3.0	ng	390747	2	8.07	2620030	20.0
n-Hexadecanoic acid	11.85	13.6	ng	1303980	4	11.31	1912560	20.0
Octadecanoic acid	12.63	20.8	ng	1629420	5	13.95	1568810	20.0
Trifluoroacetoxy ...	13.80	9.2	ng	717502	5	13.95	1568810	20.0