LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF030917\
Data File : BF093492.D
Acq On : 9 Mar 2017 23:02
Operator : SJ/MA
Sample : I2195-11
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-5-TP-4-COMP-0-12FT

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-BF030717.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	1.967	5	7	20	rVB	73200	176545	3.12%	0.358%
2	3.590	146	149	155	rBV	30457	64731	1.14%	0.131%
3	4.916	262	265	274	rBV	645885	1251266	22.10%	2.538%
4	5.350	301	303	320	rBV	4846904	5517006	97.42%	11.192%
5	5.750	336	338	345	rVB	38585	56984	1.01%	0.116%
6	6.402	393	395	398	rBV	3875348	5663103	100.00%	11.488%
7	6.527	403	406	408	rBV	4370307	5327158	94.07%	10.807%
8	6.619	413	414	423	rVB	26346	64786	1.14%	0.131%
9	6.756	423	426	428	rBV	773945	1091286	19.27%	2.214%
10	6.905	437	439	442	rBV	4151724	3863095	68.22%	7.837%
11	7.327	473	476	478	rBV	3322854	3838914	67.79%	7.788%
12	8.036	535	538	545	rVB	1584350	1480053	26.14%	3.002%
13	9.110	629	632	634	rBV	5256716	5315261	93.86%	10.783%
14	9.511	664	667	669	rBV	898197	809881	14.30%	1.643%
15	9.785	689	691	693	rBV	1691847	1582000	27.94%	3.209%
16	10.208	727	728	730	rVB	73350	78946	1.39%	0.160%
17	10.573	758	760	763	rBV2	2410654	2877287	50.81%	5.837%
18	10.688	768	770	777	rVB2	107926	238115	4.20%	0.483%
19	11.134	806	809	810	rBV	99829	103589	1.83%	0.210%
20	11.271	819	821	823	rBV	1578537	1630262	28.79%	3.307%
21	11.556	844	846	848	rBV	90470	73856	1.30%	0.150%
22	12.859	957	960	962	rBV	3539928	5105538	90.15%	10.357%
23	13.762	1036	1039	1047	rBV	105622	241800	4.27%	0.491%
24	13.911	1050	1052	1054	rBV	1516547	1560632	27.56%	3.166%
25	15.317	1172	1175	1184	rVB	1006480	1283068	22.66%	2.603%

Sum of corrected areas: 49295162

LSC Report - Integrated Chromatogram

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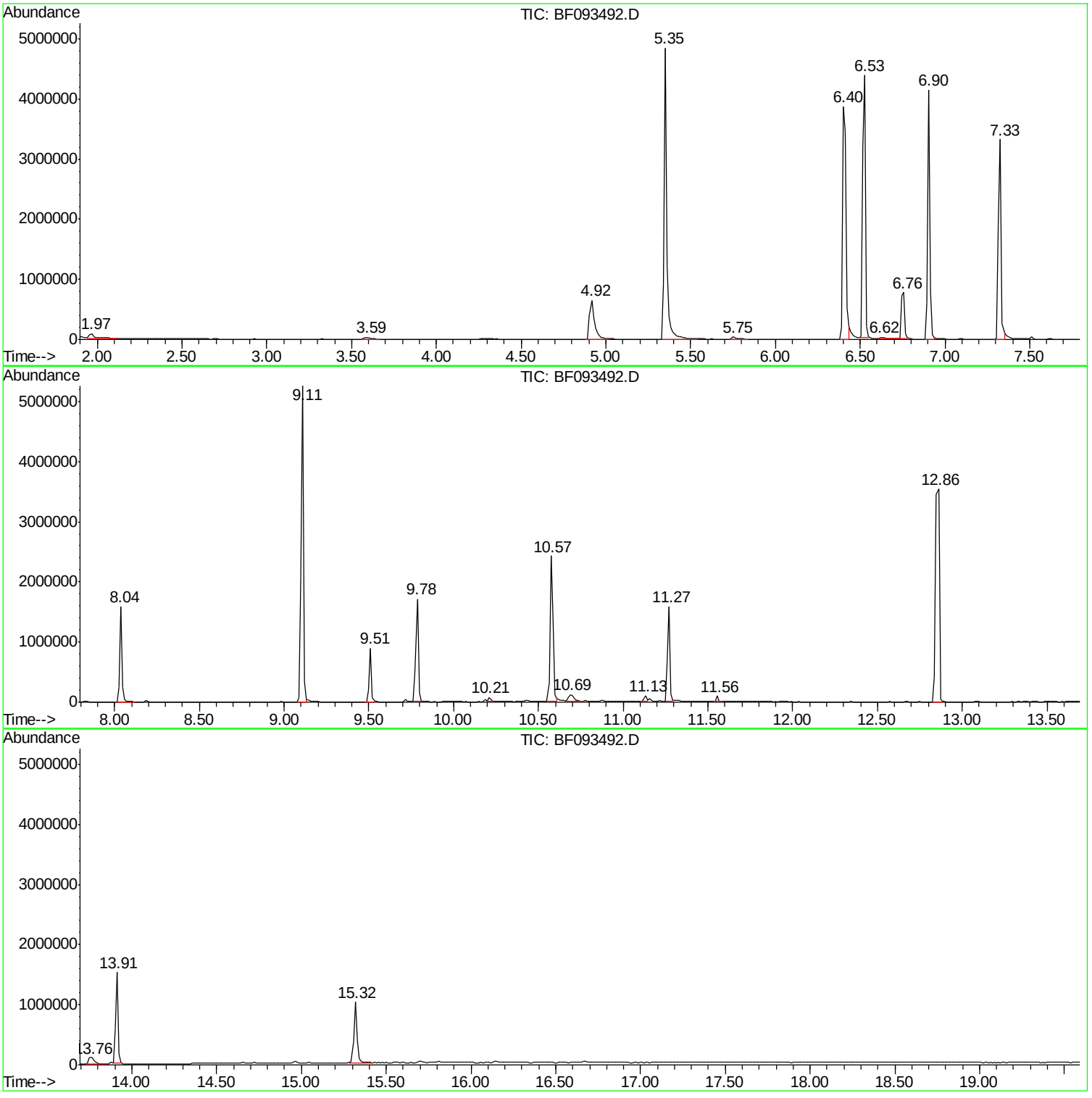
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-5-TP-4-COMP-0-12FT

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

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Sample : I2195-11
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Instrument : BNA_F
ClientSampleId : TP-5-TP-4-COMP-0-12FT

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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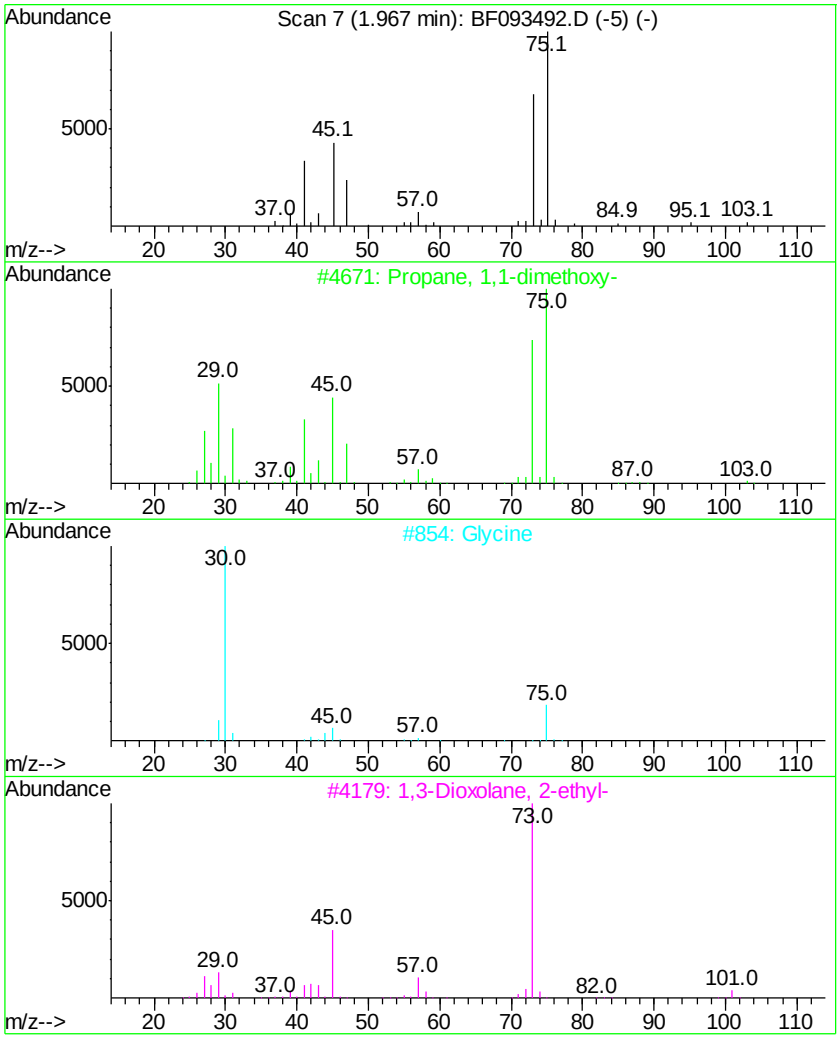
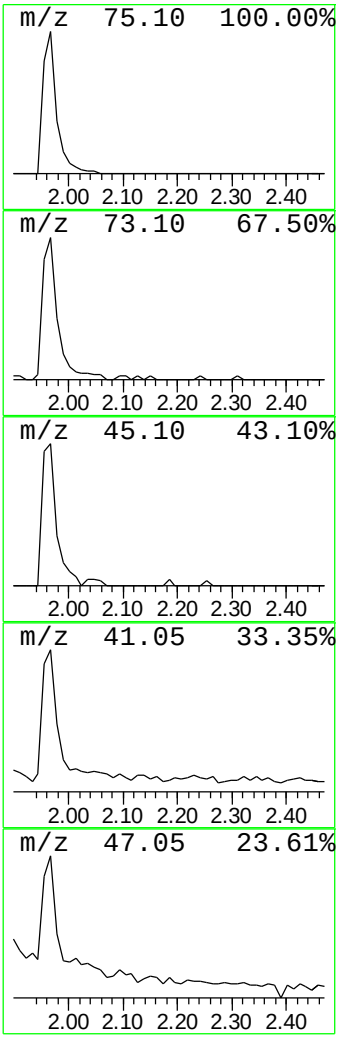
Peak Number 1 Propane, 1,1-dimethoxy- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.97	3.24 ng	176545	1,4-Dichlorobenzene-d4	6.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	83
2	Glycine	75	C2H5NO2	000056-40-6	9
3	1,3-Dioxolane, 2-ethyl-	102	C5H10O2	002568-96-9	9
4	Dodecane, 1,1-dimethoxy-	230	C14H30O2	014620-52-1	9
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9





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Instrument : BNA_F
ClientSampleId : TP-5-TP-4-COMP-0-12FT

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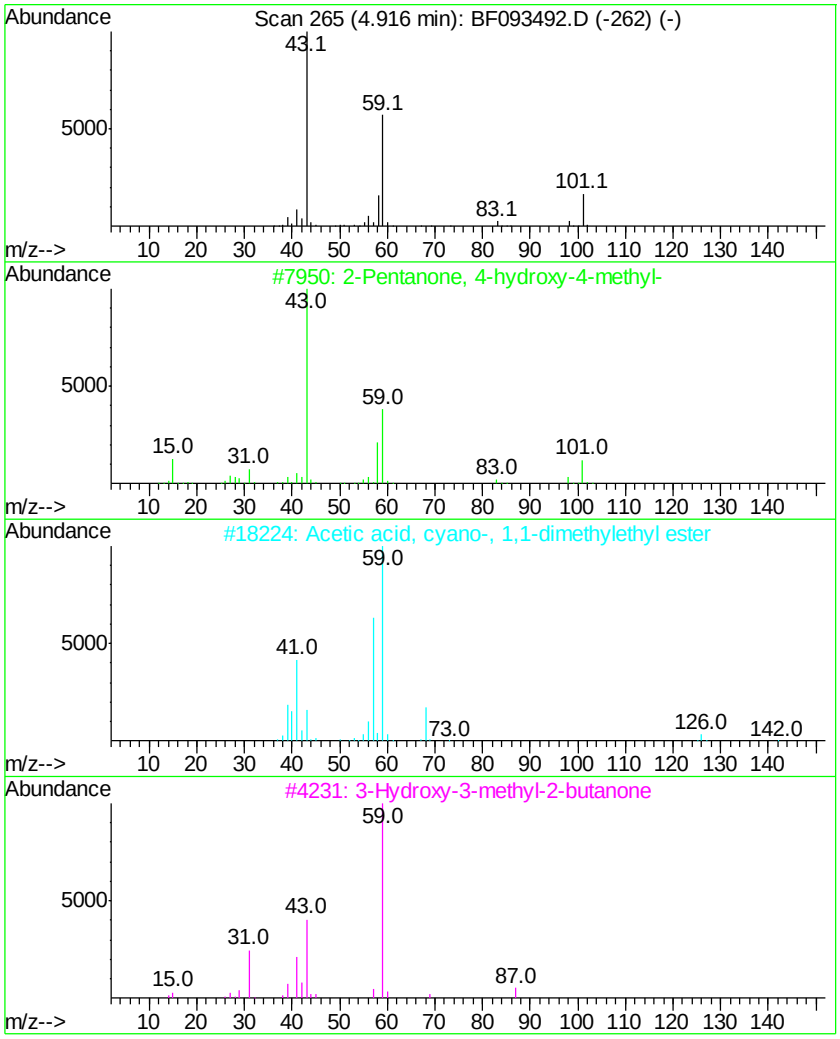
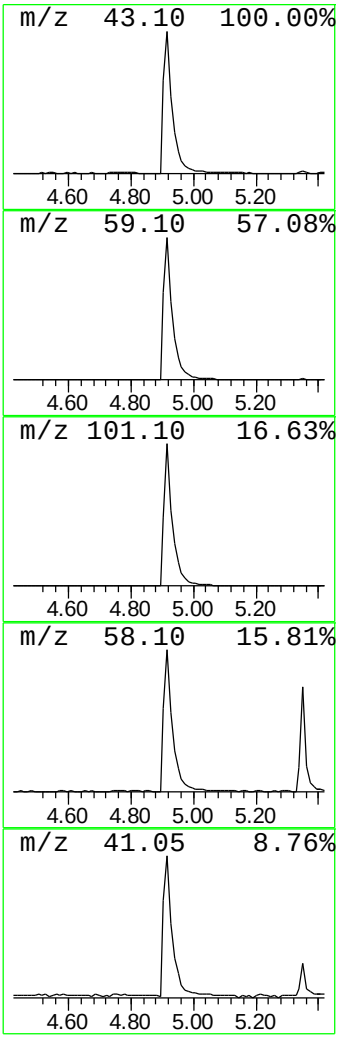
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.92	22.93 ng	1251270	1,4-Dichlorobenzene-d4	6.76

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, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9
4	5-Oxohexanenitrile	111	C6H9NO	010412-98-3	9
5	Butanamide, 2-hydroxy-2,N-dimethyl-	117	C5H11NO2	039961-72-3	9





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Operator : SJ/MA
Sample : I2195-11
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-5-TP-4-COMP-0-12FT

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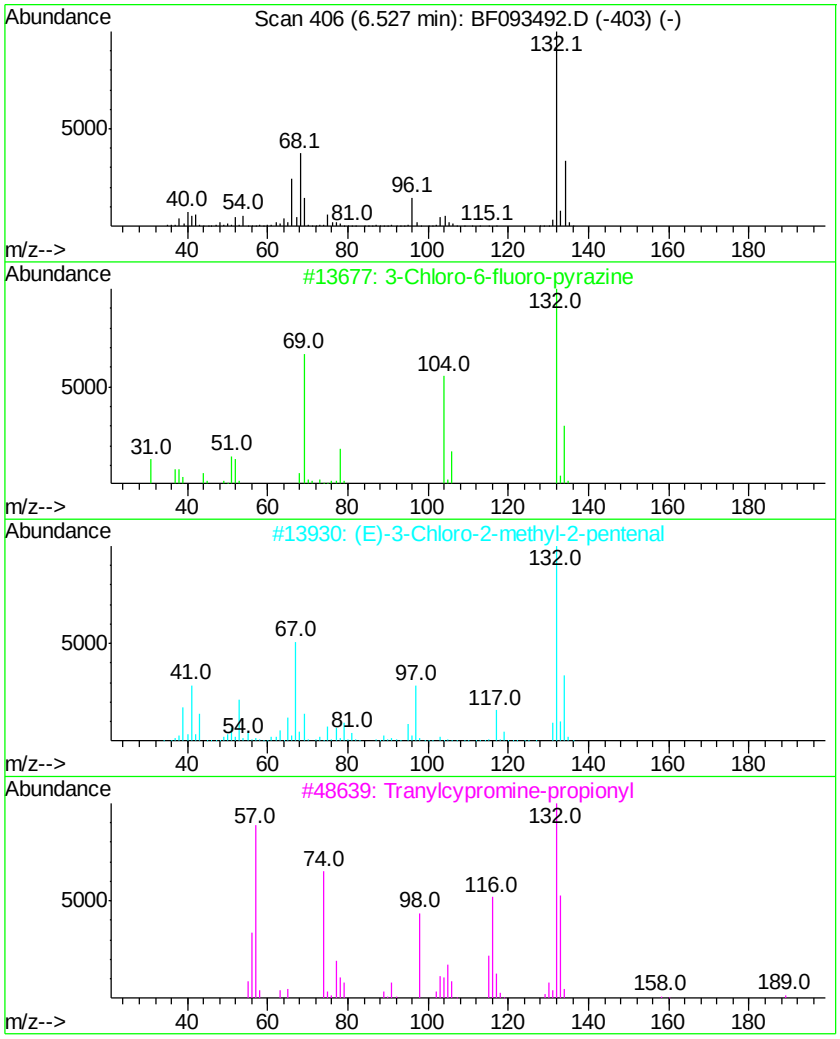
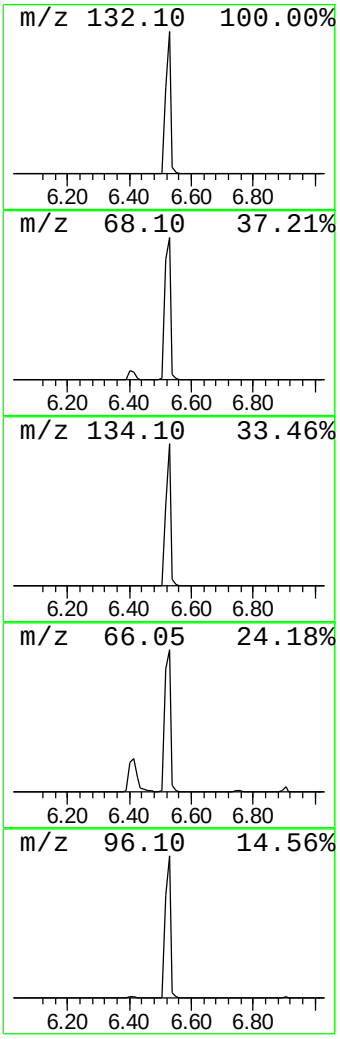
Peak Number 3 unknown6.53 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.53	97.63 ng	5327160	1,4-Dichlorobenzene-d4	6.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	16
4	5-Aminoindole	132	C8H8N2	005192-03-0	16
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





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Instrument : BNA_F
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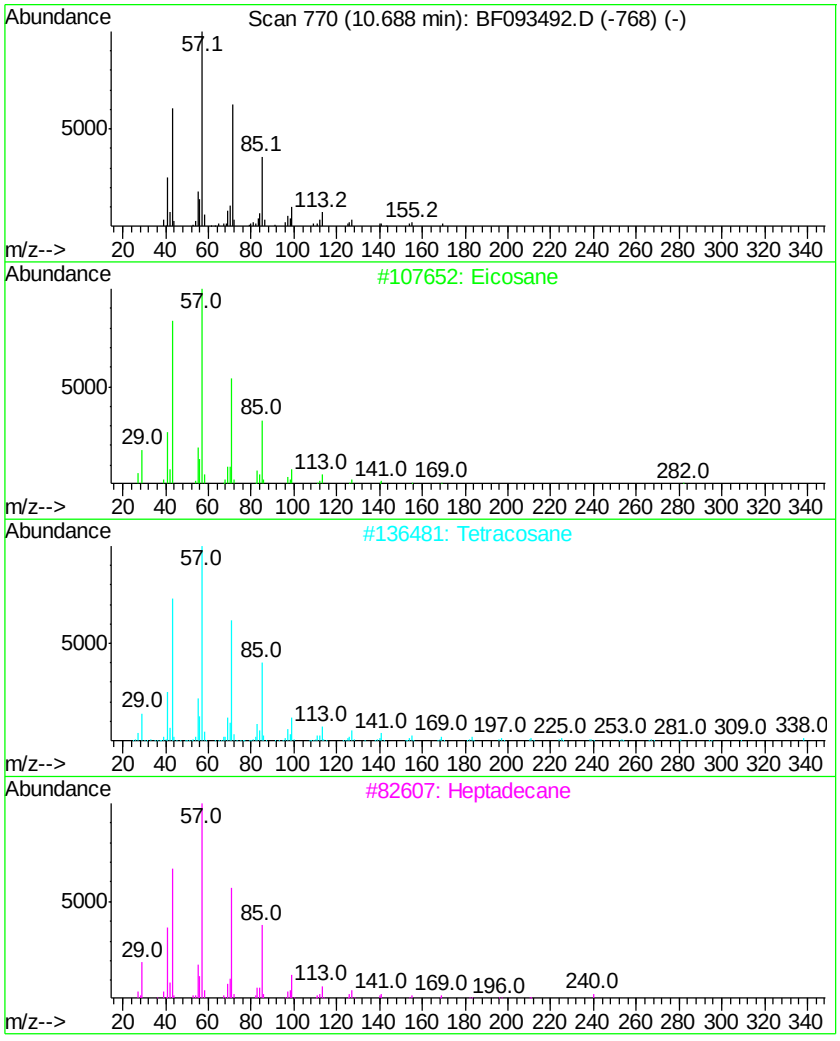
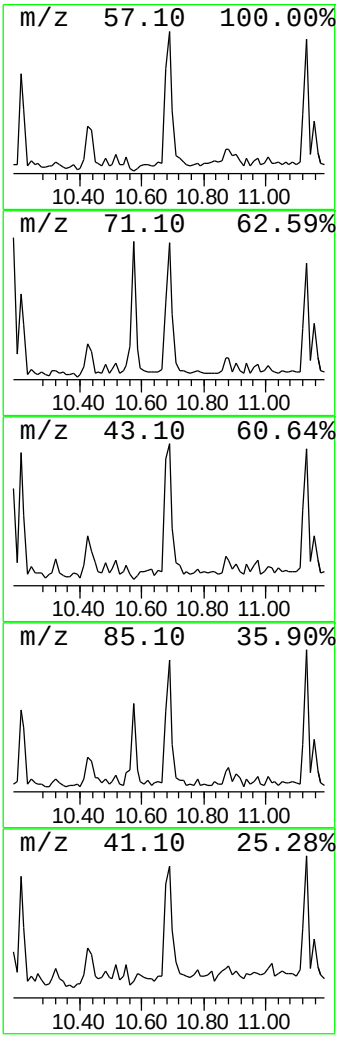
Peak Number 5 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.69	2.92 ng	238115	Phenanthrene-d10	11.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	90
2	Tetracosane	338	C24H50	000646-31-1	90
3	Heptadecane	240	C17H36	000629-78-7	90
4	Tetradecane	198	C14H30	000629-59-4	87
5	Tridecane	184	C13H28	000629-50-5	86





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Instrument :
BNA_F
ClientSampleId :
TP-5-TP-4-COMP-0-12FT

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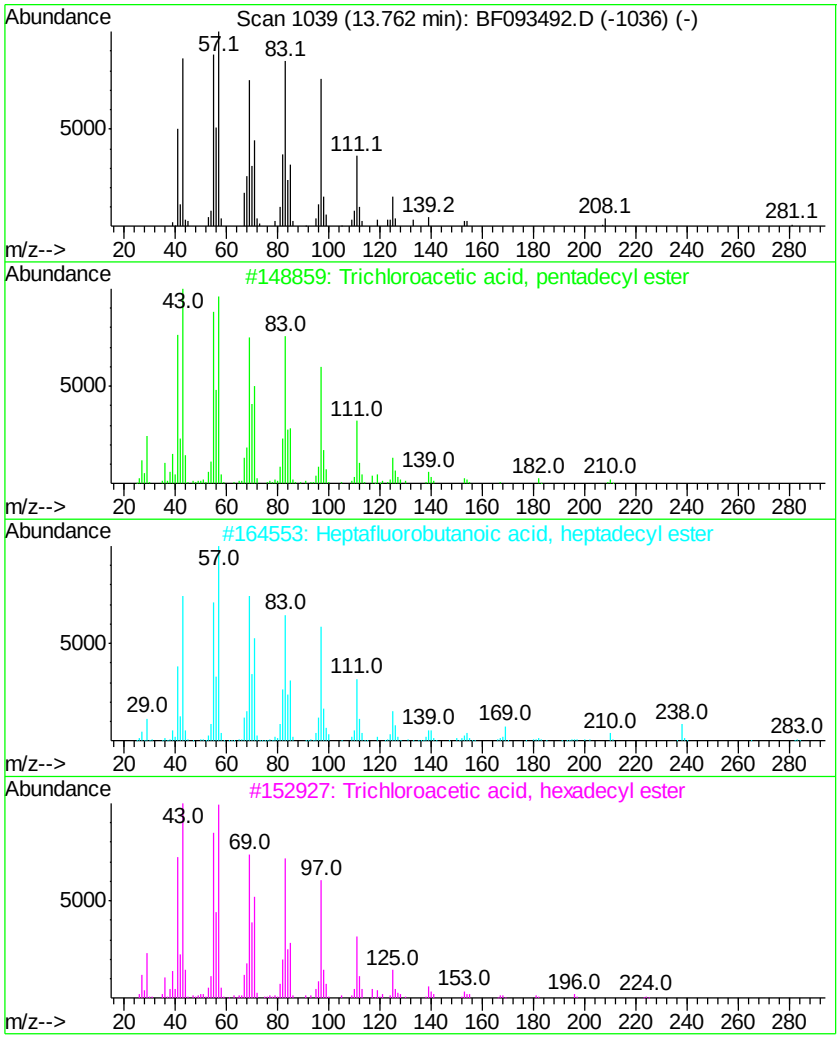
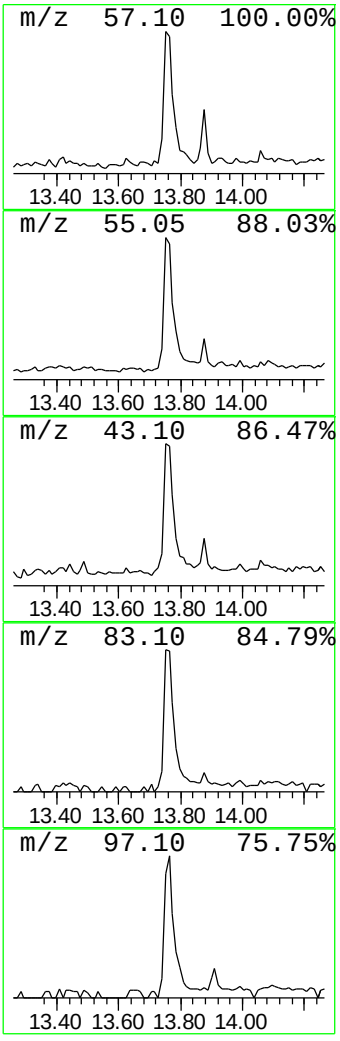
****

Peak Number 6 Trichloroacetic acid, penta... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.76	3.10 ng	241800	Chrysene-d12	13.91

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	90
2	Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	87
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	87
4	11-Tricosene	322	C23H46	052078-56-5	87
5	Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	86





Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Propane, 1,1-dime...	1.97	3.2	ng	176545	1	6.76	1091290	20.0
2-Pentanone, 4-hy...	4.92	22.9	ng	1251270	1	6.76	1091290	20.0
unknown6.53	6.53	97.6	ng	5327160	1	6.76	1091290	20.0
Eicosane	10.69	2.9	ng	238115	4	11.27	1630260	20.0
Trichloroacetic a...	13.76	3.1	ng	241800	5	13.91	1560630	20.0