LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF020817\
Data File : BF092868.D
Acq On : 8 Feb 2017 22:08
Operator : SJ/MA
Sample : I1741-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 020617-PR-E-D-M

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	4.407	201	203	213	rVB	162776	227789	4.72%	0.778%
2	5.059	258	260	263	rBV	1067739	1130798	23.43%	3.860%
3	5.493	295	298	300	rBV	1005205	1039087	21.53%	3.547%
4	5.893	330	333	335	rBV	195110	168990	3.50%	0.577%
5	6.522	386	388	392	rBV	768534	754841	15.64%	2.577%
6	6.659	398	400	402	rBV	2219521	1875918	38.87%	6.404%
7	6.887	418	420	423	rBV	613073	825063	17.10%	2.817%
8	7.047	432	434	437	rBV	2850508	2844974	58.95%	9.712%
9	7.459	467	470	472	rBV	2543733	2436961	50.49%	8.319%
10	8.179	530	533	535	rBV	1321393	1165944	24.16%	3.980%
11	9.253	624	627	630	rBV	4194895	4246457	87.99%	14.496%
12	9.642	659	661	663	rBV	134328	164710	3.41%	0.562%
13	9.928	684	686	689	rBV	1299693	1254961	26.00%	4.284%
14	10.362	720	724	725	rBV	72400	86899	1.80%	0.297%
15	10.716	753	755	758	rBV	1487469	1588823	32.92%	5.424%
16	10.831	763	765	770	rVB	109237	130672	2.71%	0.446%
17	11.276	803	804	810	rVB	66504	99509	2.06%	0.340%
18	11.413	814	816	819	rBV	1351717	1298950	26.91%	4.434%
19	13.002	952	955	958	rBV	3369125	4826166	100.00%	16.475%
20	13.905	1031	1034	1044	rBV	99557	229893	4.76%	0.785%
21	14.054	1044	1047	1050	rVB	1432353	1334023	27.64%	4.554%
22	15.505	1170	1174	1179	rBV	839564	1225130	25.39%	4.182%
23	15.940	1209	1212	1217	rBV	46165	72736	1.51%	0.248%
24	16.431	1252	1255	1261	rBV2	52819	103694	2.15%	0.354%
25	17.003	1301	1305	1309	rVB	26085	54666	1.13%	0.187%
26	17.688	1361	1365	1369	rVB3	19618	55875	1.16%	0.191%
27	18.488	1429	1435	1440	rBV6	13077	49462	1.02%	0.169%

Sum of corrected areas: 29292991

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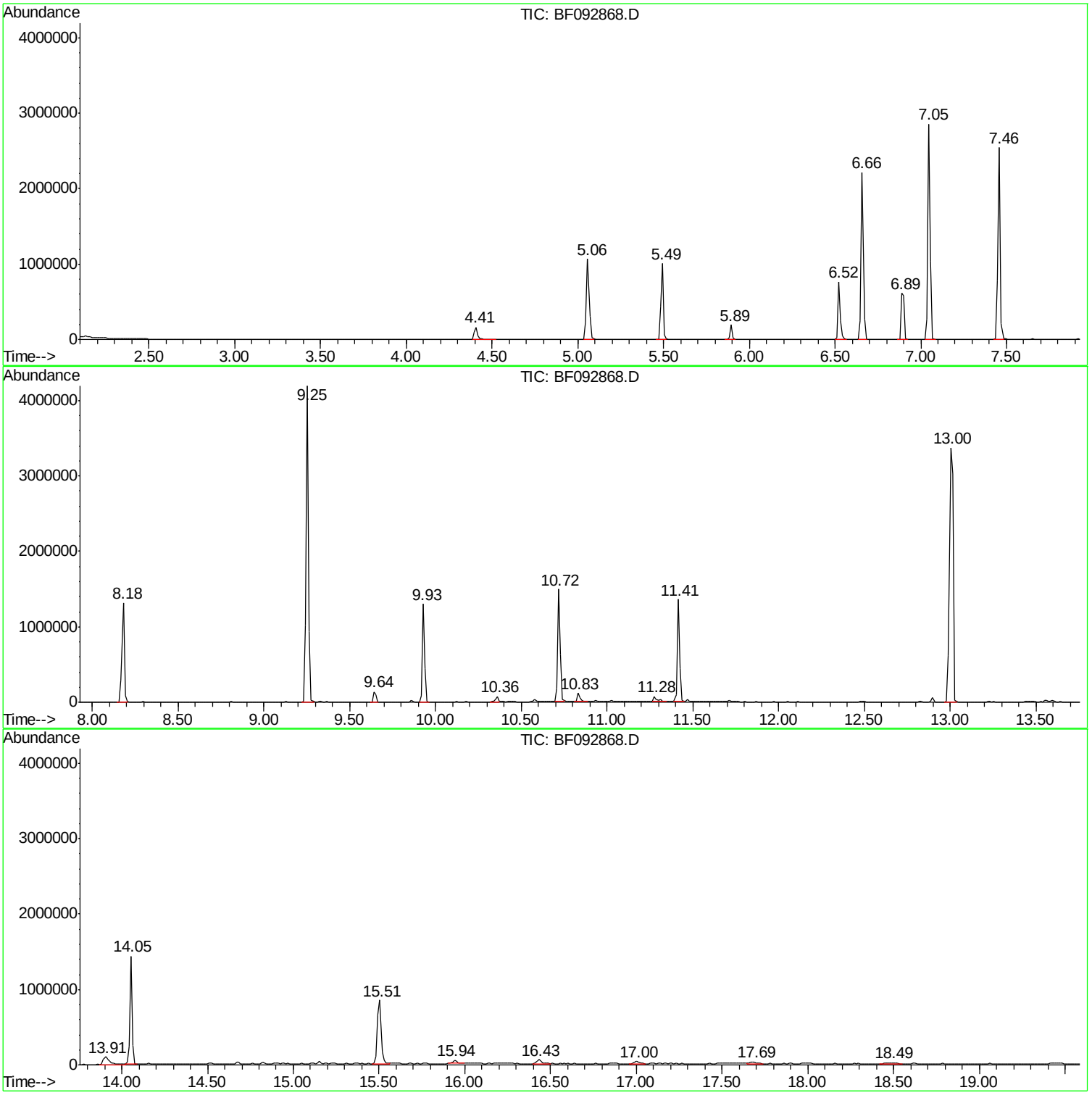
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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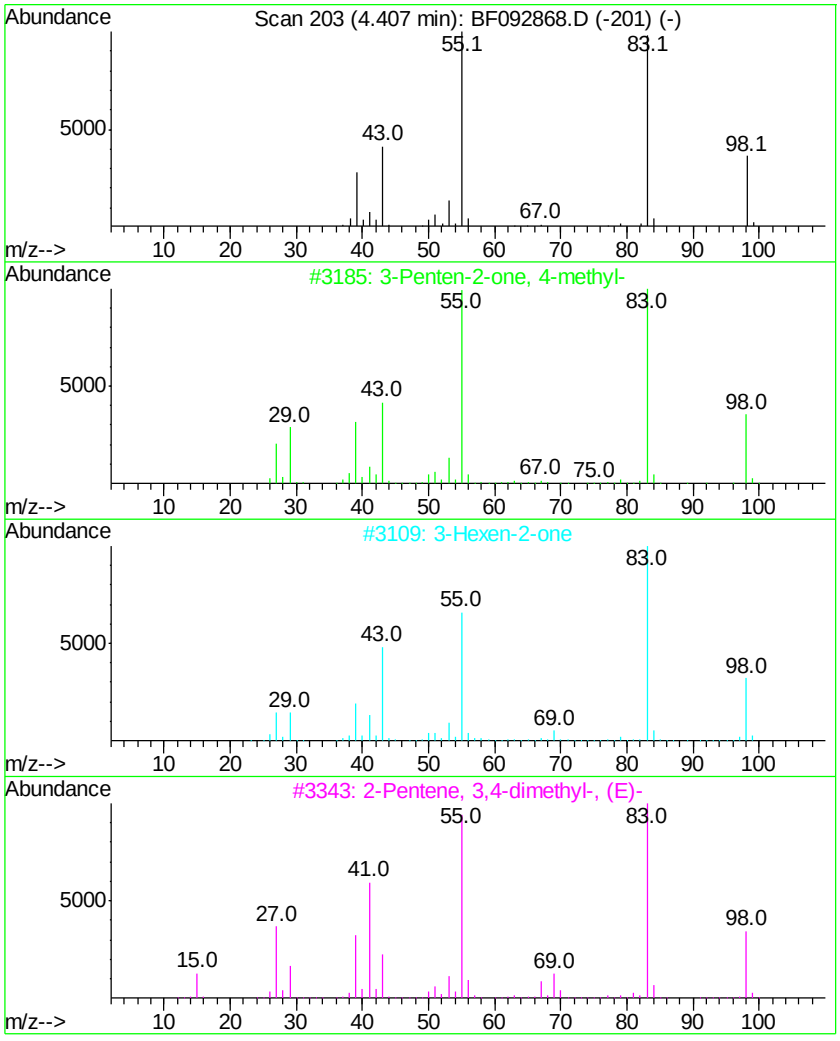
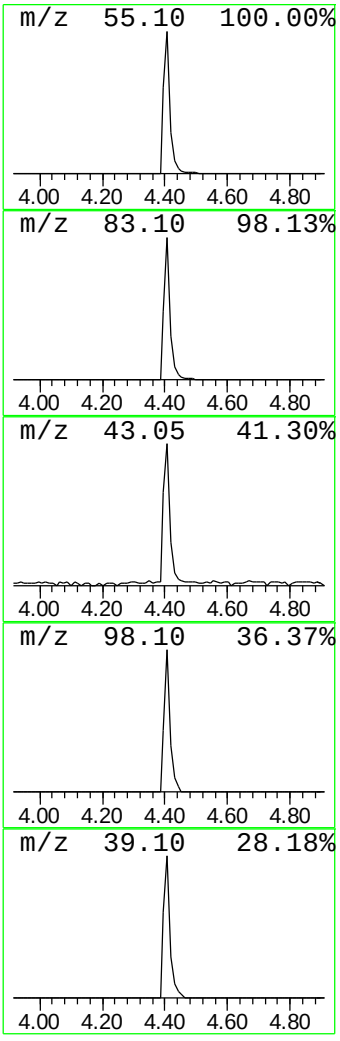
Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.41	5.52 ng	227789	1,4-Dichlorobenzene-d4	6.90

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	90
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, 2,4-dimethyl-	98	C7H14	000625-65-0	80





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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
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TIC Integration Parameters: LSCINT.P

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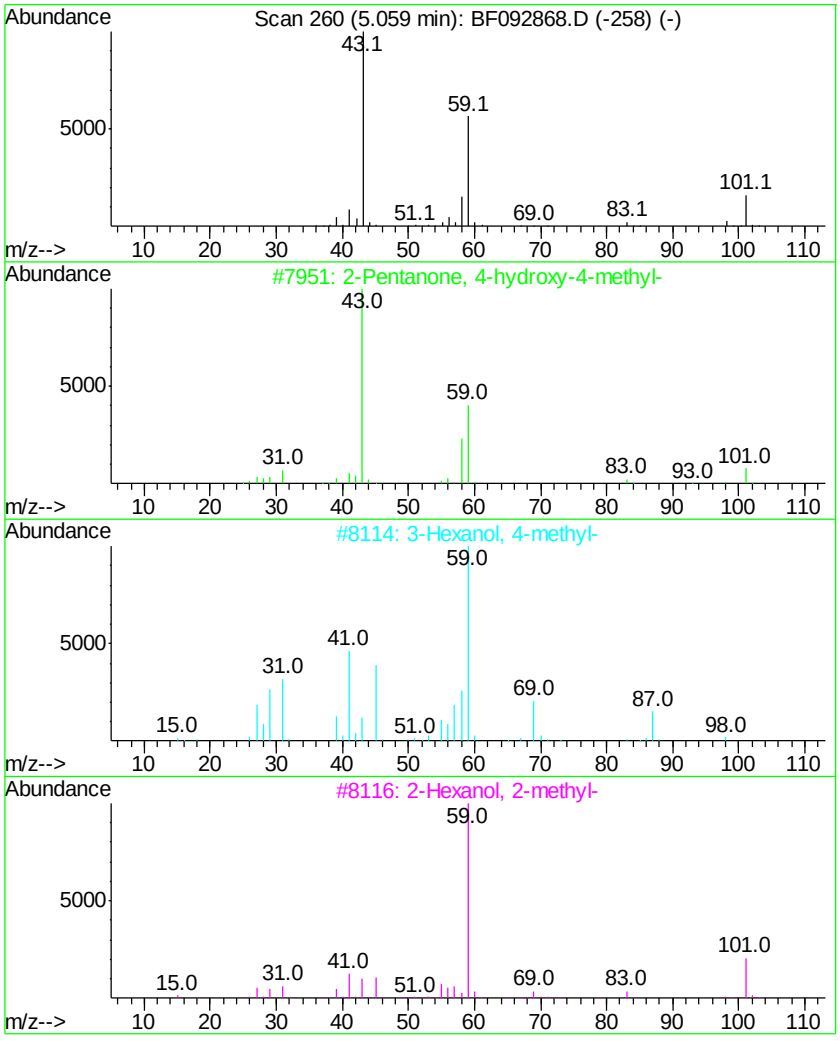
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.06	27.41 ng	1130800	1,4-Dichlorobenzene-d4	6.90

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, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



m/z 43.10 100.00%
m/z 59.10 56.56%
m/z 101.10 15.88%
m/z 58.10 15.23%
m/z 41.10 8.88%

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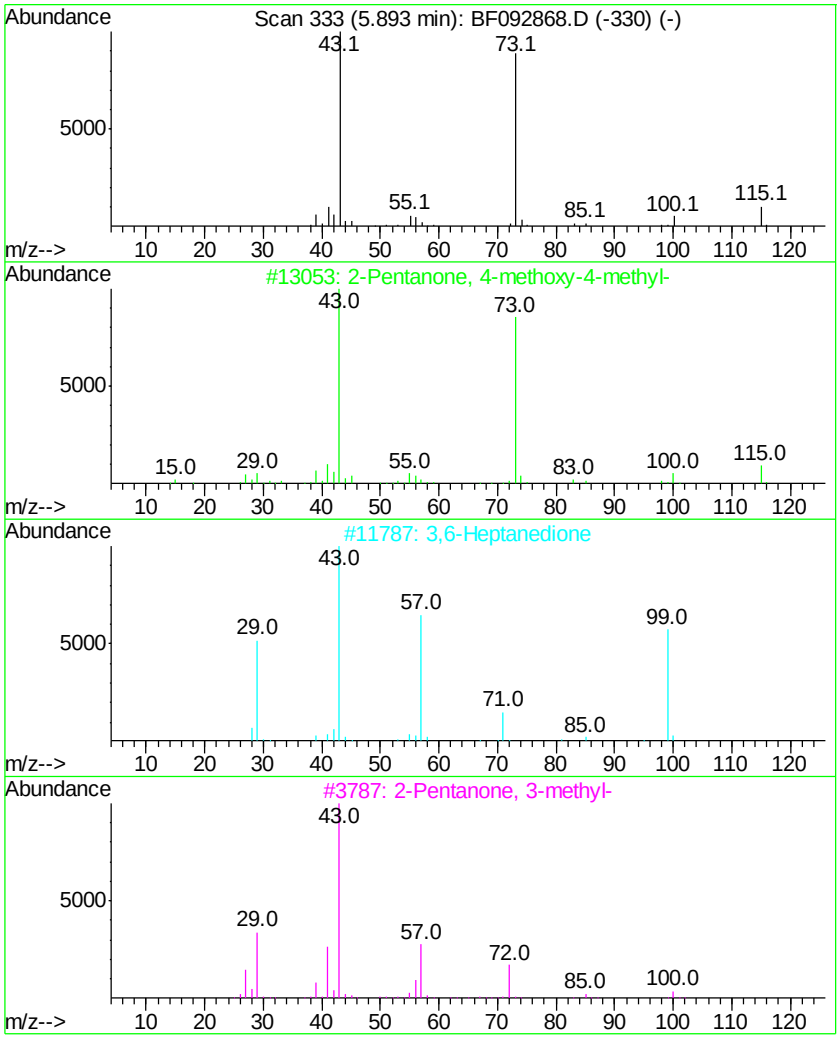
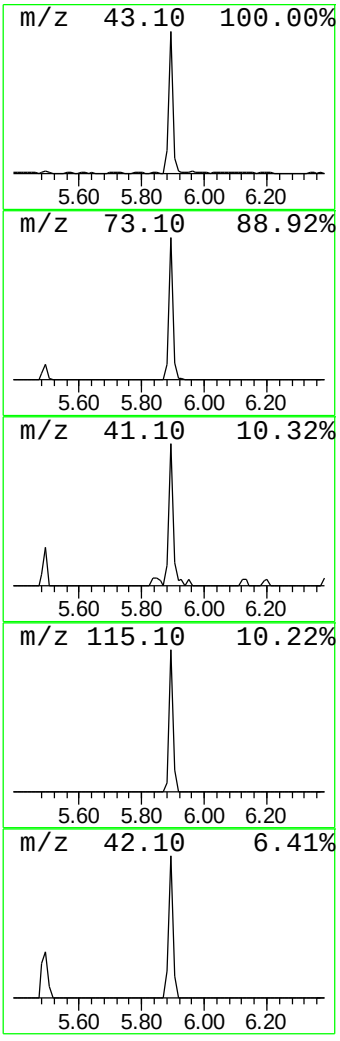
Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.89	4.10 ng	168990	1,4-Dichlorobenzene-d4	6.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2	3,6-Heptanedione	128	C7H12O2	001703-51-1	12
3	2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	10
4	2-Pentene, 2-methoxy-	100	C6H12O	061142-47-0	9
5	Hexane, 2-methyl-	100	C7H16	000591-76-4	9





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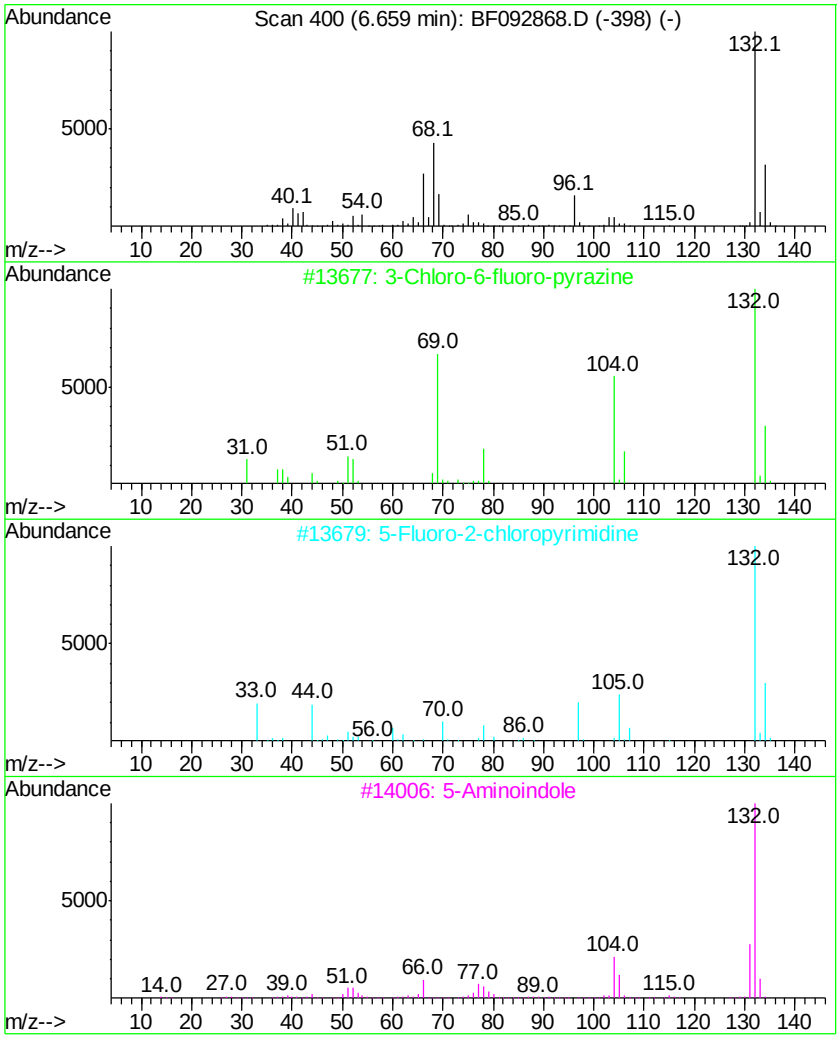
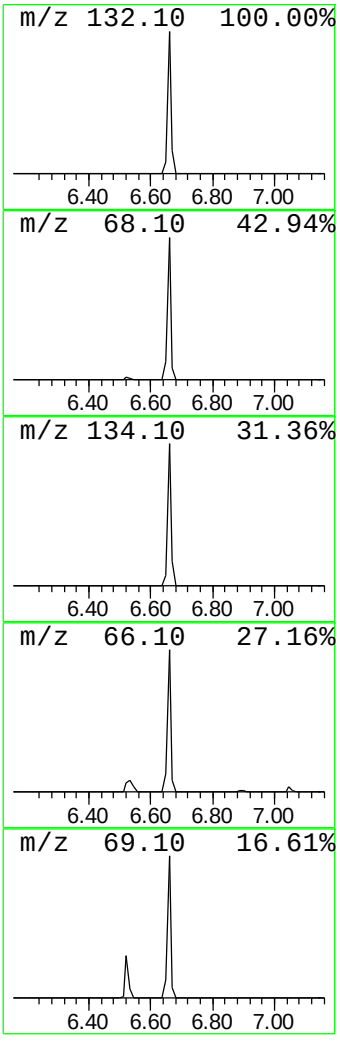
Peak Number 4 unknown6.66 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	45.47 ng	1875920	1,4-Dichlorobenzene-d4	6.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9





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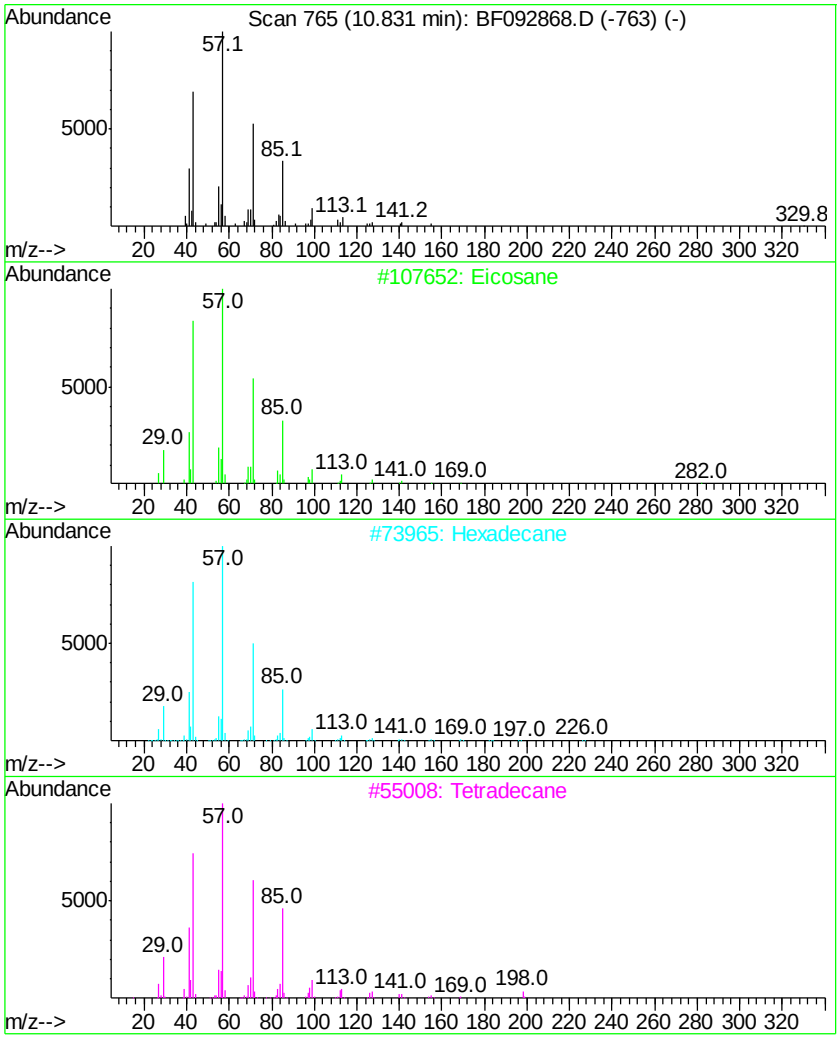
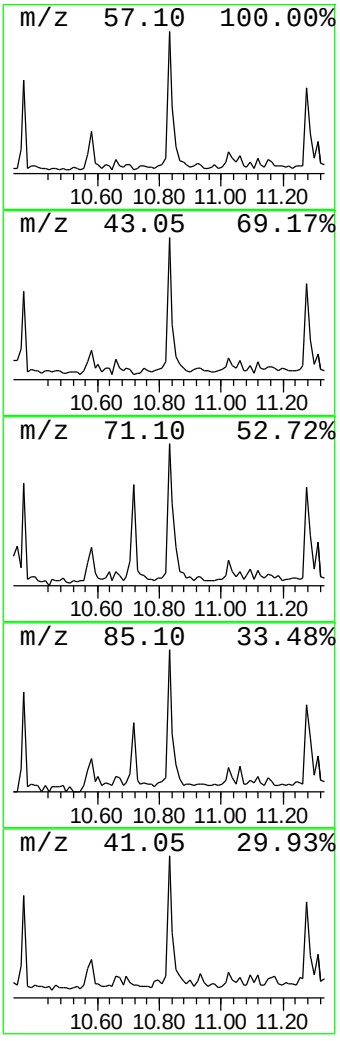
Peak Number 6 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.83	2.01 ng	130672	Phenanthrene-d10	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	91
2	Hexadecane	226	C16H34	000544-76-3	90
3	Tetradecane	198	C14H30	000629-59-4	90
4	Pentadecane	212	C15H32	000629-62-9	90
5	Heptadecane	240	C17H36	000629-78-7	90





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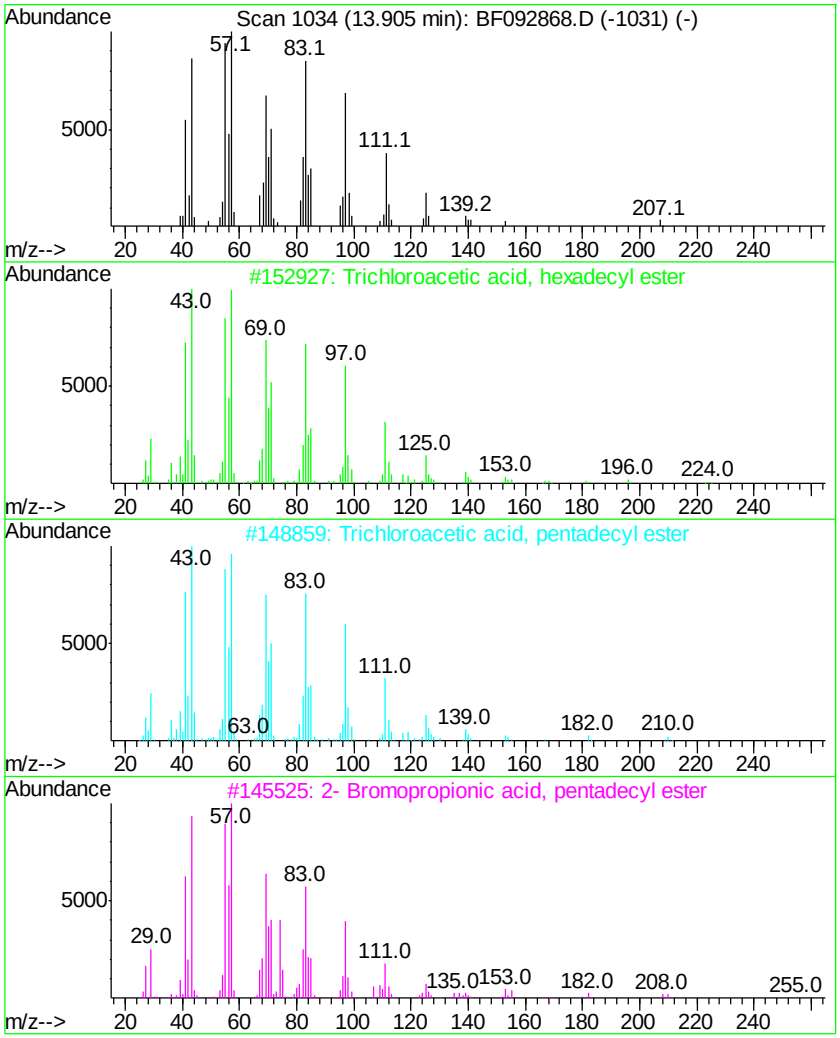
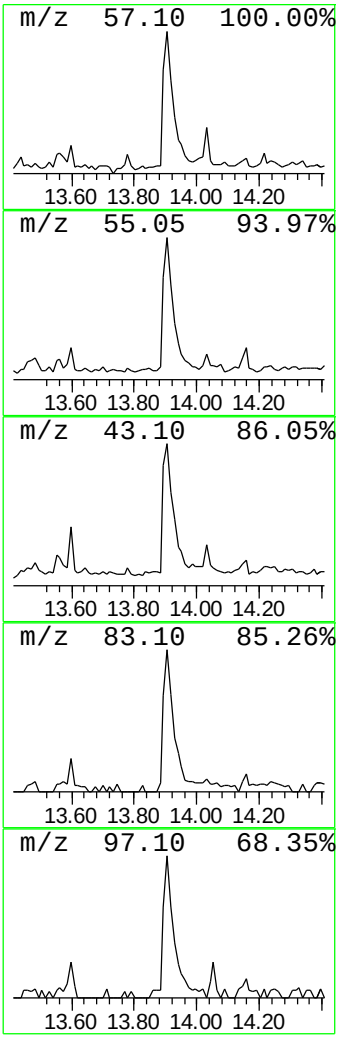
Peak Number 7 Trichloroacetic acid, hexad... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.91	3.45 ng	229893	Chrysene-d12	14.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
2	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
3	2- Bromopropionic acid, pentadec...	362	C18H35BrO2	1000292-44-2	91
4	1-Docosene	308	C22H44	001599-67-3	91
5	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	91





Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
3-Penten-2-one, 4...	4.41	5.5	ng	227789	1	6.90	825063	20.0
2-Pentanone, 4-hy...	5.06	27.4	ng	1130800	1	6.90	825063	20.0
2-Pentanone, 4-me...	5.89	4.1	ng	168990	1	6.90	825063	20.0
unknown6.66	6.66	45.5	ng	1875920	1	6.90	825063	20.0
Eicosane	10.83	2.0	ng	130672	4	11.41	1298950	20.0
Trichloroacetic a...	13.91	3.5	ng	229893	5	14.05	1334020	20.0