LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF021317\
Data File : BF092932.D
Acq On : 13 Feb 2017 21:40
Operator : SJ/MA
Sample : I1799-06
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SW-3

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	5.047	257	259	270	rBV	367200	501123	9.23%	1.372%
2	5.482	295	297	300	rBV	1817402	1654047	30.45%	4.530%
3	6.510	385	387	391	rBV	1131015	1047088	19.28%	2.868%
4	6.647	396	399	402	rBV	3091025	2882175	53.06%	7.893%
5	6.876	417	419	422	rBV	755590	820575	15.11%	2.247%
6	7.036	431	433	436	rBV	3193112	2960766	54.50%	8.109%
7	7.447	466	469	471	rBV	2641820	2579960	47.49%	7.066%
8	7.550	474	478	484	rBV	74057	134563	2.48%	0.369%
9	7.905	506	509	513	rBV3	30250	62158	1.14%	0.170%
10	8.053	520	522	524	rBV3	26272	55576	1.02%	0.152%
11	8.168	530	532	534	rVB	1256988	1171493	21.57%	3.208%
12	8.499	559	561	563	rBV2	54398	72414	1.33%	0.198%
13	8.533	563	564	574	rVB	45325	90103	1.66%	0.247%
14	9.242	623	626	628	rBV	4650487	4693540	86.40%	12.854%
15	9.916	683	685	687	rBV	1463911	1320142	24.30%	3.615%
16	10.316	718	720	724	rBV	173140	208027	3.83%	0.570%
17	10.705	751	754	757	rBV	2408752	2452545	45.15%	6.717%
18	10.819	762	764	768	rVB	56063	81894	1.51%	0.224%
19	11.402	812	815	817	rBV	1301590	1319424	24.29%	3.614%
20	12.739	930	932	935	rBV3	36778	66932	1.23%	0.183%
21	12.808	935	938	940	rVV	4892530	5432176	100.00%	14.877%
22	12.991	951	954	956	rBV	3987320	4437802	81.69%	12.154%
23	13.894	1030	1033	1039	rBV3	25257	64831	1.19%	0.178%
24	14.031	1043	1045	1048	rVB	1122155	1216525	22.39%	3.332%
25	14.660	1098	1100	1105	rBV3	40664	81690	1.50%	0.224%
26	15.471	1168	1171	1174	rBV	811571	1106115	20.36%	3.029%

Sum of corrected areas: 36513684

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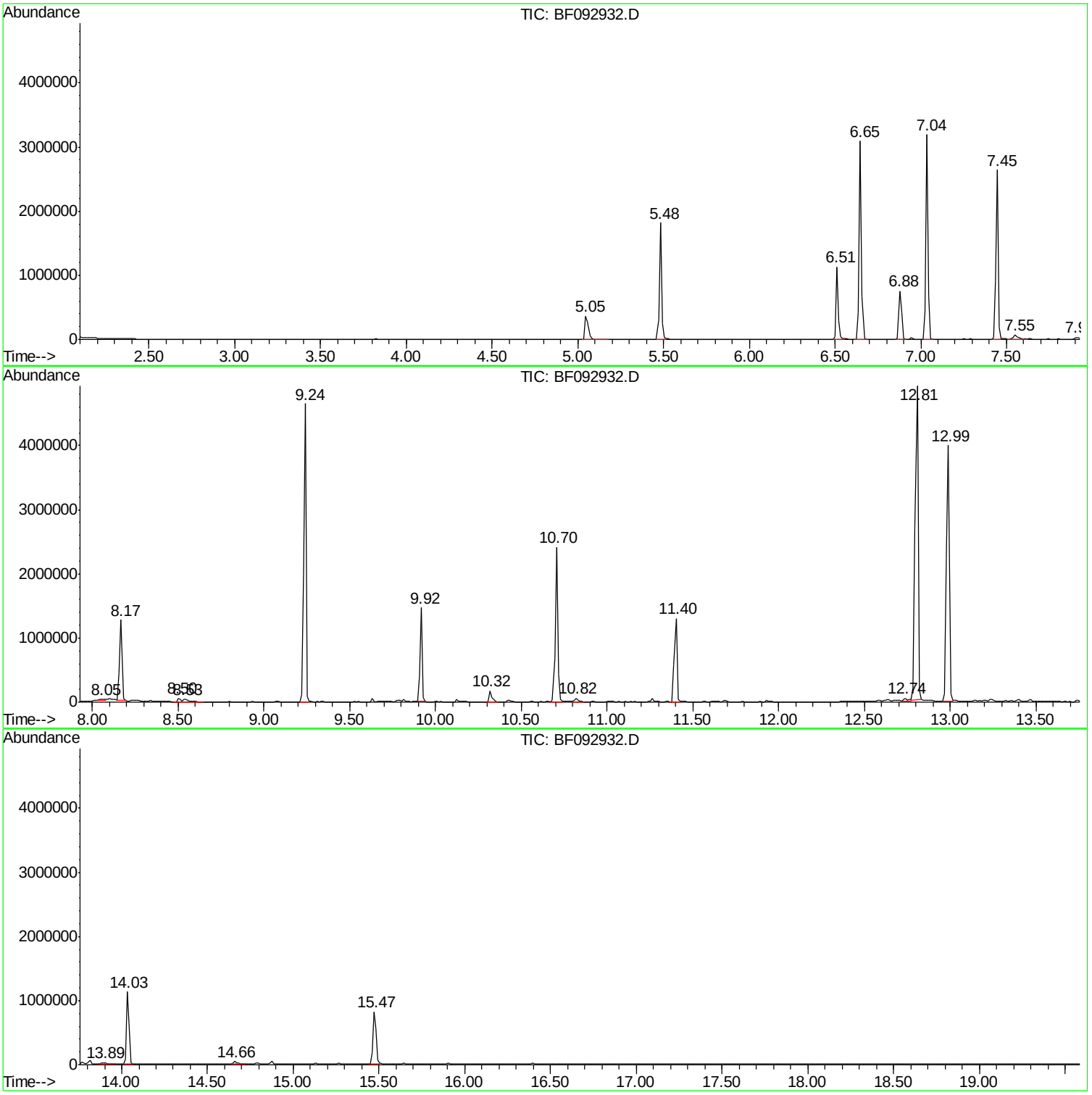
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

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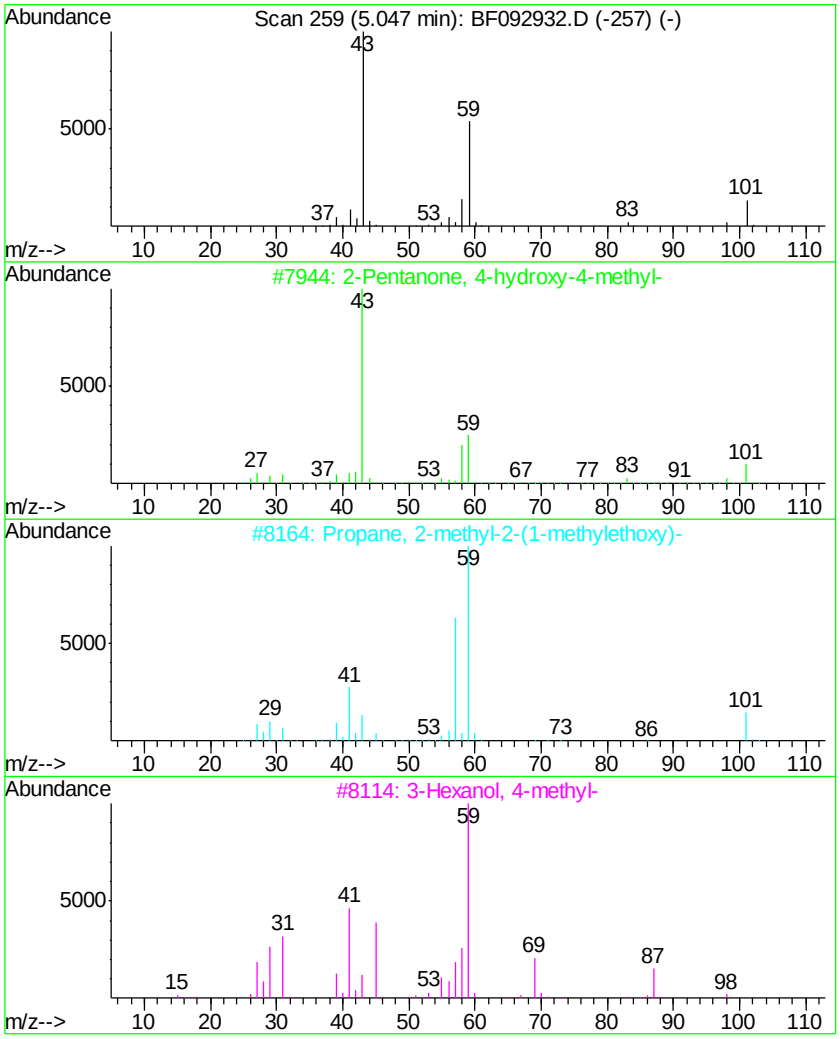
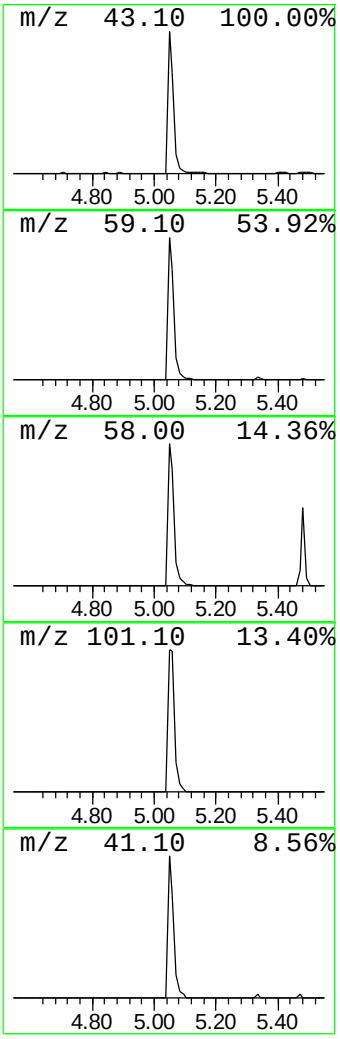
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.05	12.21 ng	501123	1,4-Dichlorobenzene-d4	6.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23





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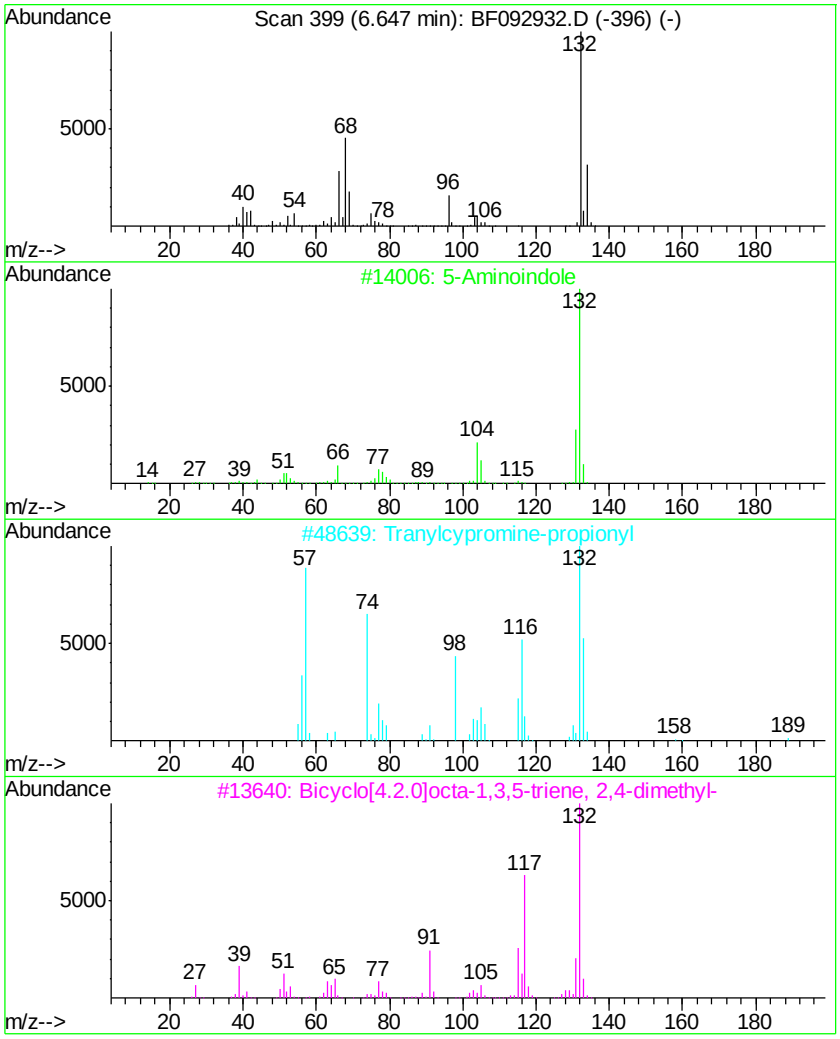
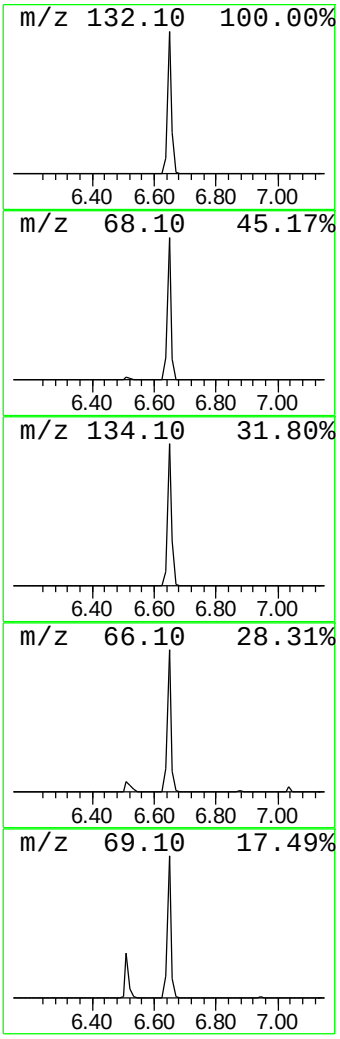
Peak Number 2 unknown6.65 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	70.25 ng	2882180	1,4-Dichlorobenzene-d4	6.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Aminoindole	132	C8H8N2	005192-03-0	12
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9





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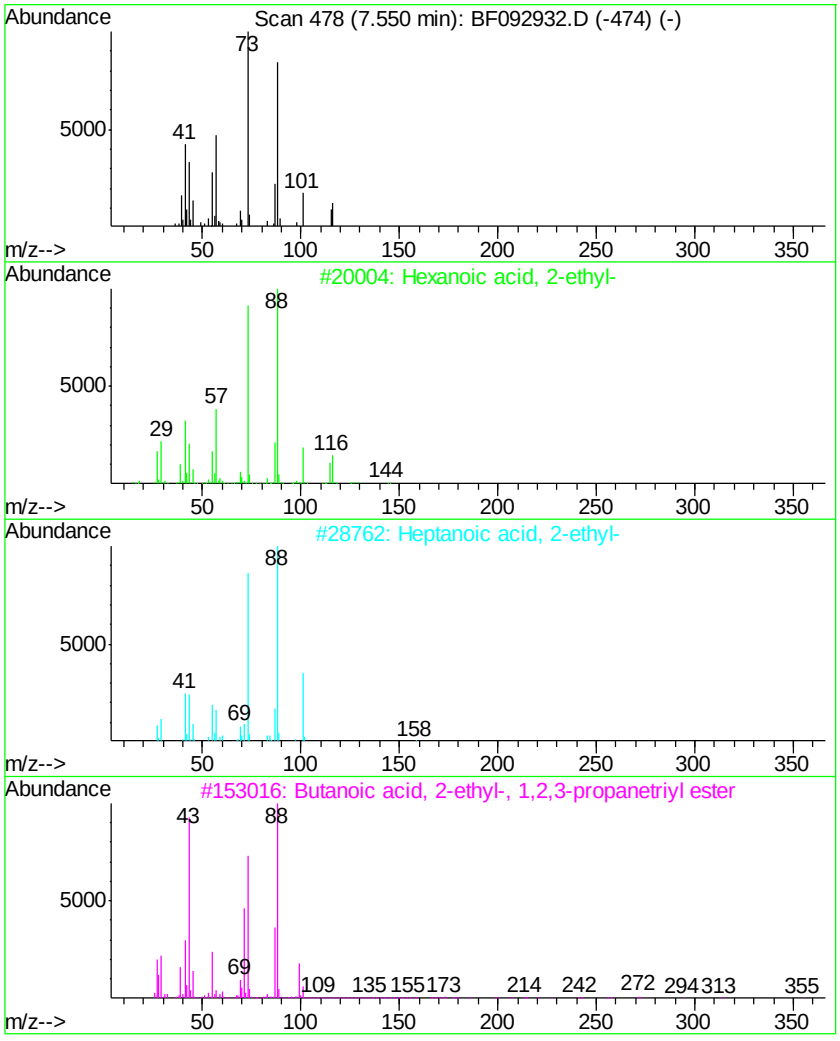
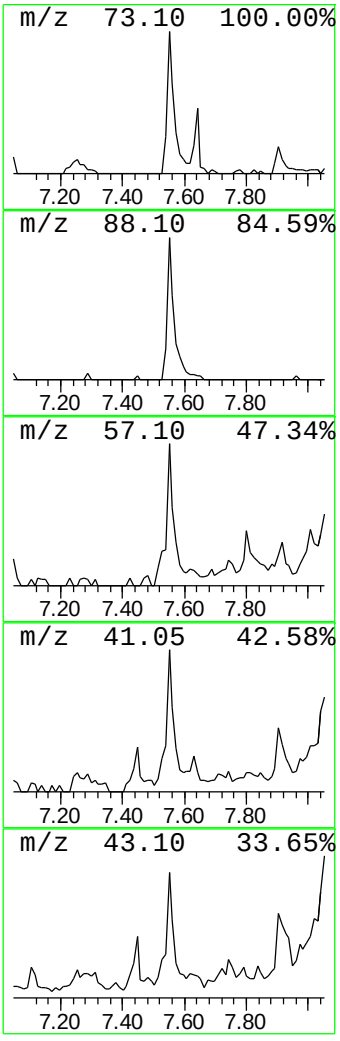
Peak Number 4 Hexanoic acid, 2-ethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.55	2.30 ng	134563	Naphthalene-d8	8.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	86
2	Heptanoic acid, 2-ethyl-	158	C9H18O2	003274-29-1	53
3	Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	53
4	Ethanamine, N-methyl-N-nitroso-	88	C3H8N2O	010595-95-6	43
5	Butanoic acid, 2-methyl-, methyl...	116	C6H12O2	000868-57-5	38





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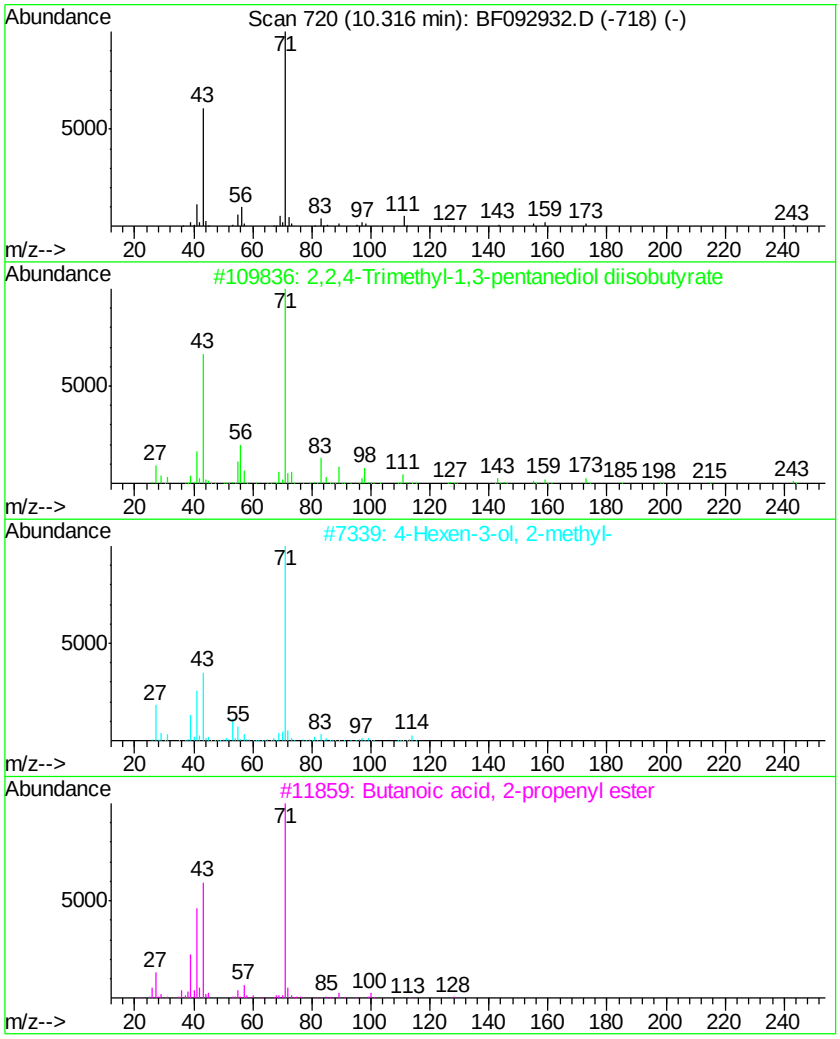
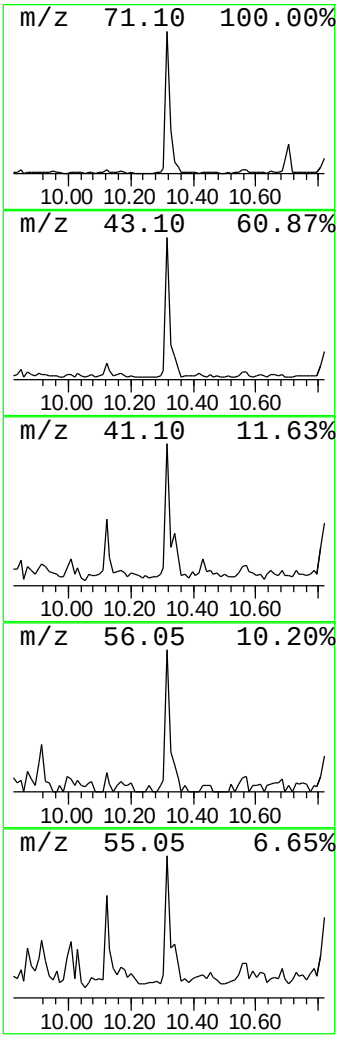
Peak Number 5 2,2,4-Trimethyl-1,3-pentane... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.32	3.15 ng	208027	Acenaphthene-d10	9.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2,4-Trimethyl-1,3-pentanediol ...	286	C16H30O4	006846-50-0	64
2	4-Hexen-3-ol, 2-methyl-	114	C7H14O	004798-60-1	59
3	Butanoic acid, 2-propenyl ester	128	C7H12O2	002051-78-7	53
4	2-Furanmethanol, tetrahydro-, ac...	144	C7H12O3	000637-64-9	53
5	Butanoic acid, 2-butoxy-1-methyl...	216	C11H20O4	007492-70-8	50





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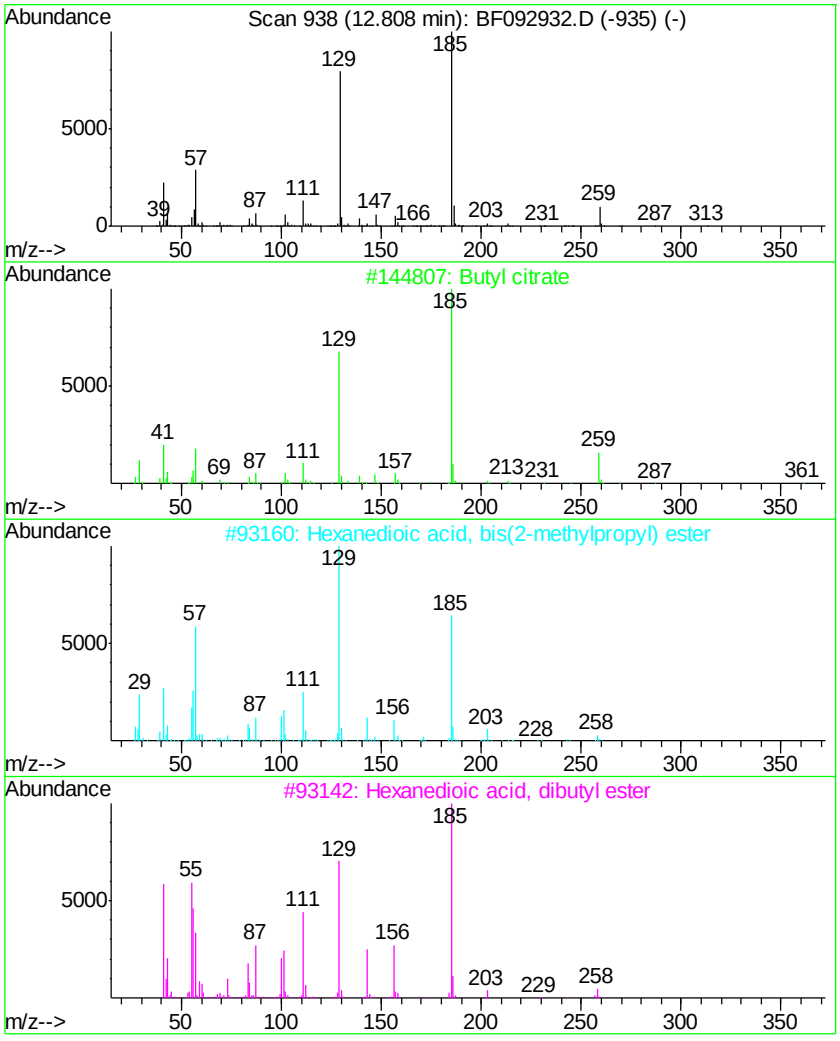
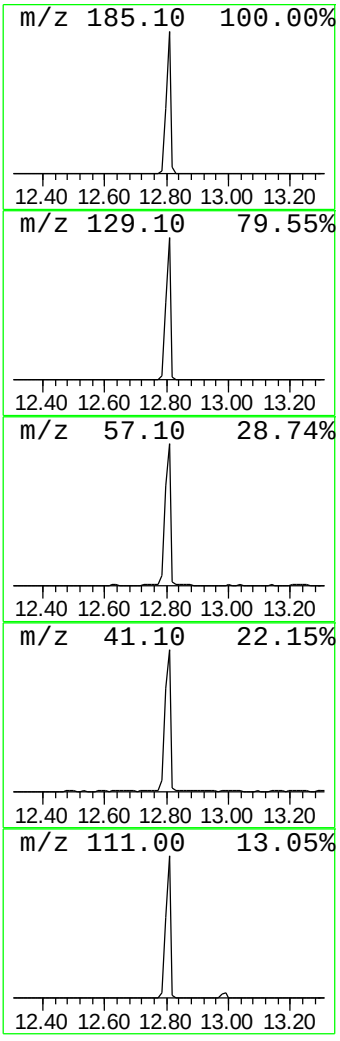
Peak Number 6 Butyl citrate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.81	89.31 ng	5432180	Chrysene-d12	14.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butyl citrate	360	C18H32O7	000077-94-1	91
2	Hexanedioic acid, bis(2-methylpr...	258	C14H26O4	000141-04-8	56
3	Hexanedioic acid, dibutyl ester	258	C14H26O4	000105-99-7	56
4	Adipic acid, di(oct-4-yl ester)	370	C22H42O4	1000160-80-1	35
5	Resorufin	213	C12H7NO3	000635-78-9	32





Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.05	12.2	ng	501123	1	6.88	820575	20.0
unknown6.65	6.65	70.3	ng	2882180	1	6.88	820575	20.0
Hexanoic acid, 2-...	7.55	2.3	ng	134563	2	8.17	1171490	20.0
2,2,4-Trimethyl-1...	10.32	3.1	ng	208027	3	9.92	1320140	20.0
Butyl citrate	12.81	89.3	ng	5432180	5	14.03	1216530	20.0