LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090515\
Data File : BF081481.D
Acq On : 6 Sep 2015 00:02
Operator : UM/IZ
Sample : G3555-06
Misc :
ALS Vial : 58 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-6

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-BF090115.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	3.541	168	171	180	rVB	13128	31387	1.68%	0.187%
2	4.410	244	247	265	rVB	668635	1251327	66.96%	7.457%
3	4.913	288	291	293	rBV	1603563	1845733	98.77%	10.999%
4	6.022	386	388	391	rBV	1275951	1868649	100.00%	11.136%
5	6.124	395	397	399	rBV	1940498	1754323	93.88%	10.454%
6	6.353	415	417	420	rVB	396152	345065	18.47%	2.056%
7	6.513	429	431	433	rBV	1411184	1277739	68.38%	7.614%
8	6.936	465	468	470	rBV	1177333	1202798	64.37%	7.168%
9	7.645	528	530	532	rBV	509529	432719	23.16%	2.579%
10	8.730	622	625	627	rBV	1812447	1737428	92.98%	10.354%
11	9.130	658	660	663	rBV	403531	366991	19.64%	2.187%
12	9.382	680	682	685	rVB	464273	433972	23.22%	2.586%
13	9.828	718	721	722	rBV2	18686	20956	1.12%	0.125%
14	10.171	748	751	753	rBV	1168269	1151728	61.63%	6.863%
15	10.319	762	764	770	rVB	27348	31800	1.70%	0.190%
16	10.765	801	803	804	rBV	21714	18983	1.02%	0.113%
17	10.845	808	810	813	rBV	483244	451619	24.17%	2.691%
18	11.428	858	861	865	rBV	68667	81969	4.39%	0.488%
19	12.296	934	937	939	rBV	115615	150216	8.04%	0.895%
20	12.365	942	943	946	rVB	22239	20001	1.07%	0.119%
21	12.434	946	949	951	rBV	1572053	1441357	77.13%	8.589%
22	12.994	995	998	1000	rBV	104777	105222	5.63%	0.627%
23	13.359	1028	1030	1036	rBV	64981	131540	7.04%	0.784%
24	13.451	1036	1038	1041	rVV	345347	322275	17.25%	1.920%
25	13.679	1056	1058	1060	rBV	24952	27346	1.46%	0.163%
26	13.977	1082	1084	1086	rBV	29034	26111	1.40%	0.156%
27	14.274	1107	1110	1112	rBV	20845	22417	1.20%	0.134%
28	14.765	1150	1153	1155	rBV	178210	229197	12.27%	1.366%

Sum of corrected areas: 16780868

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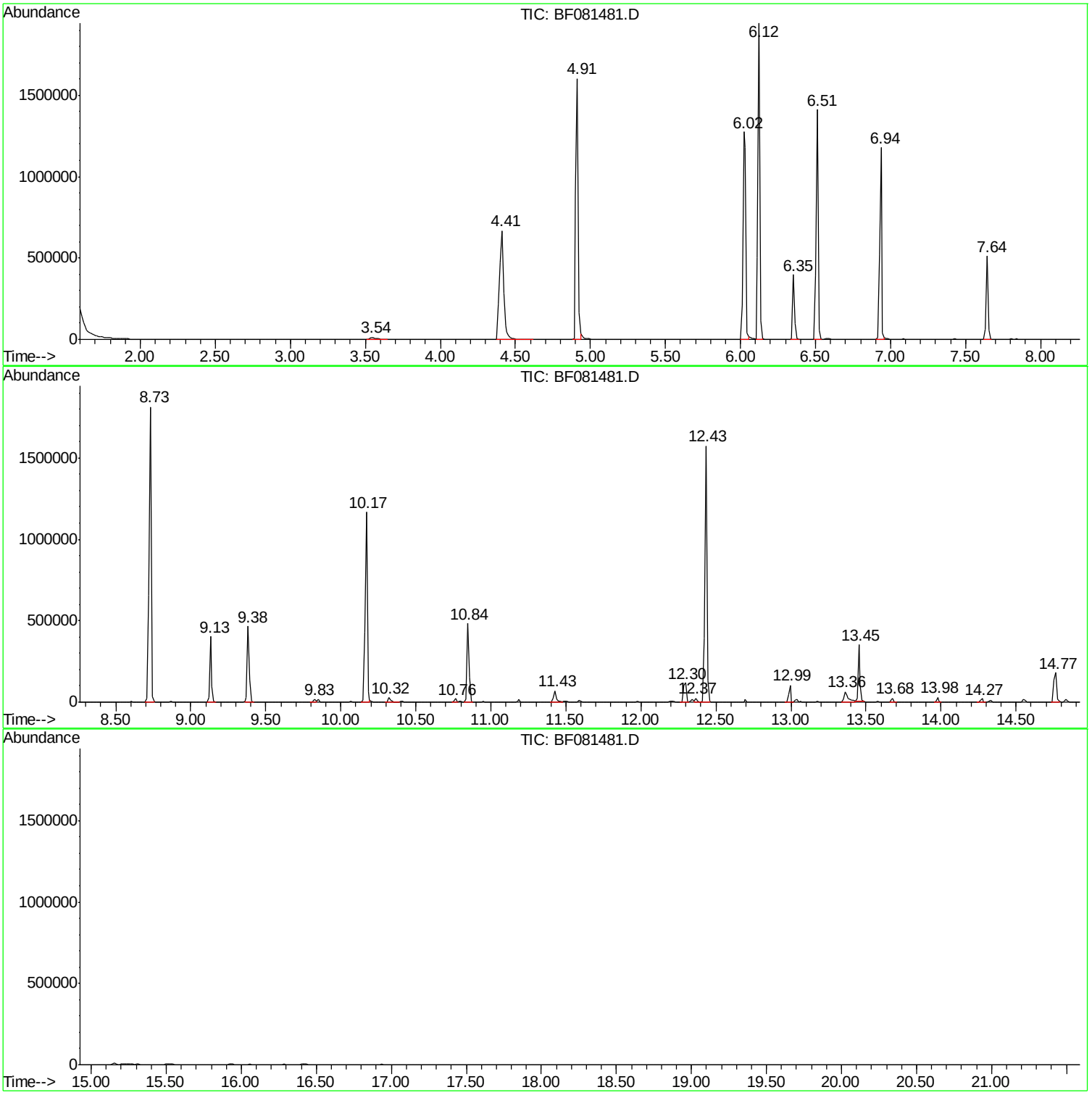
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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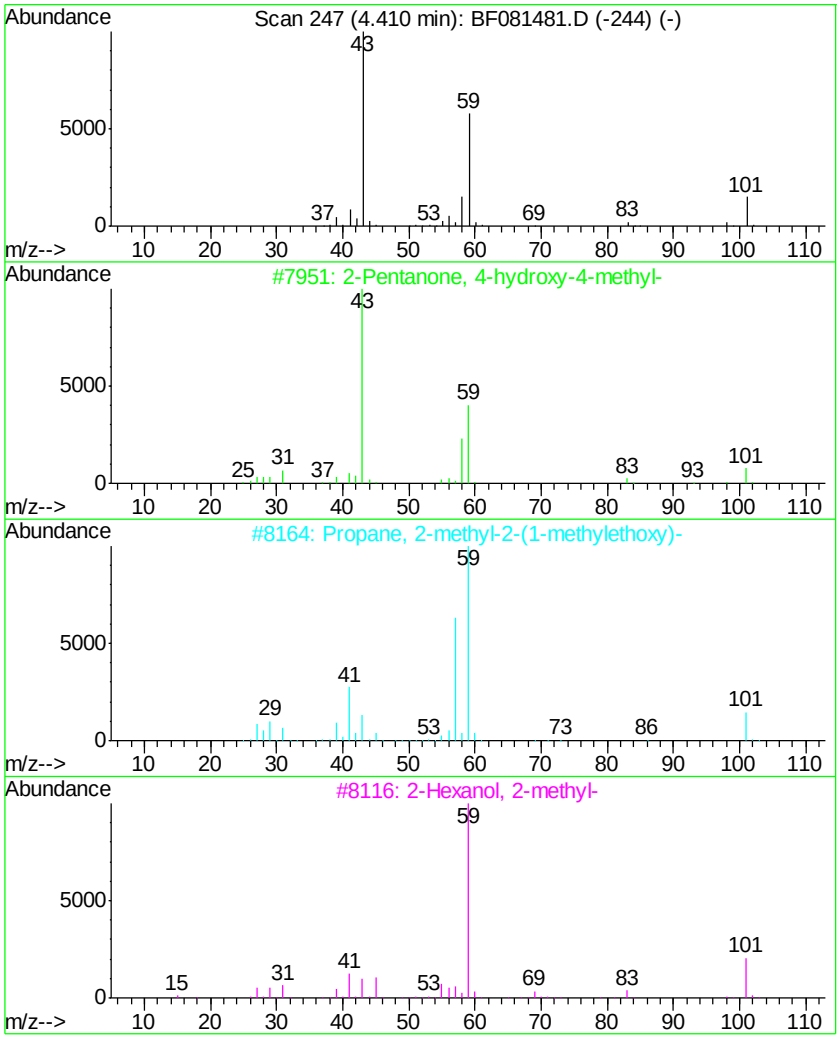
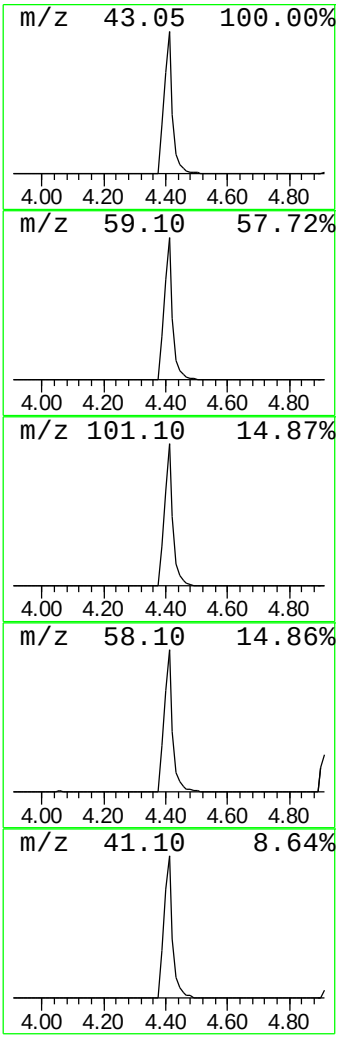
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.41	72.53 ng	1251330	1,4-Dichlorobenzene-d4	6.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23





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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
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TIC Library : C:\DATABASE\NIST02.L
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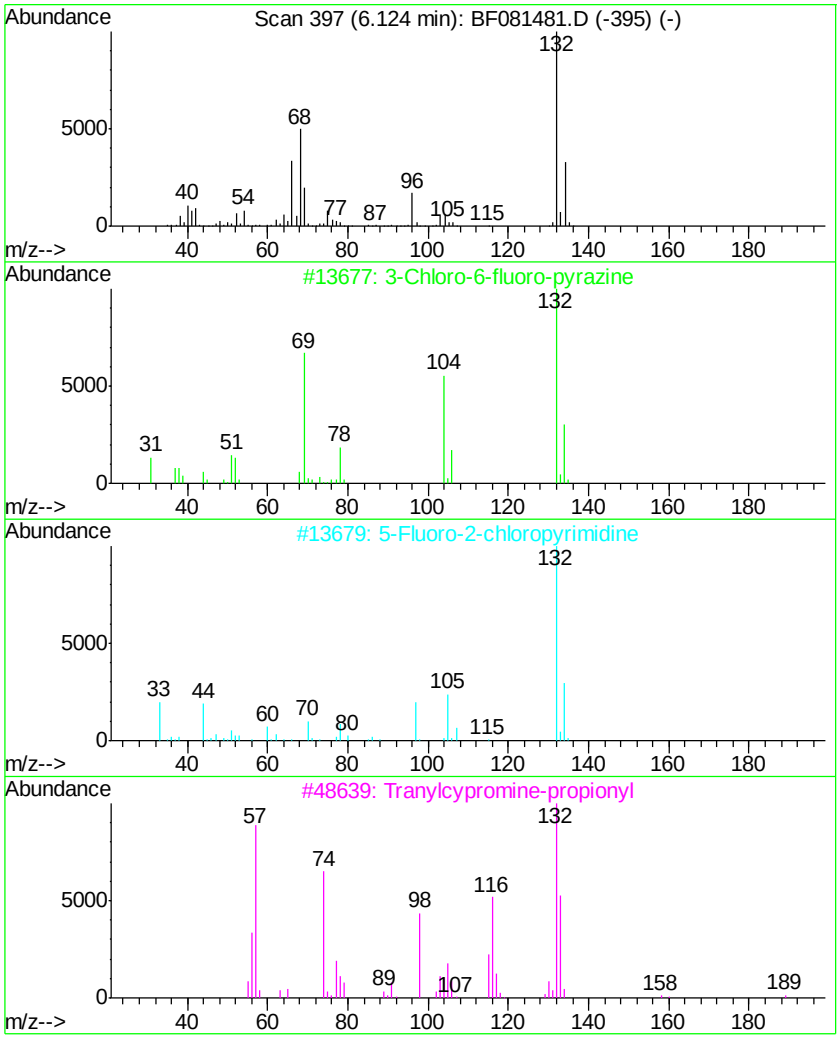
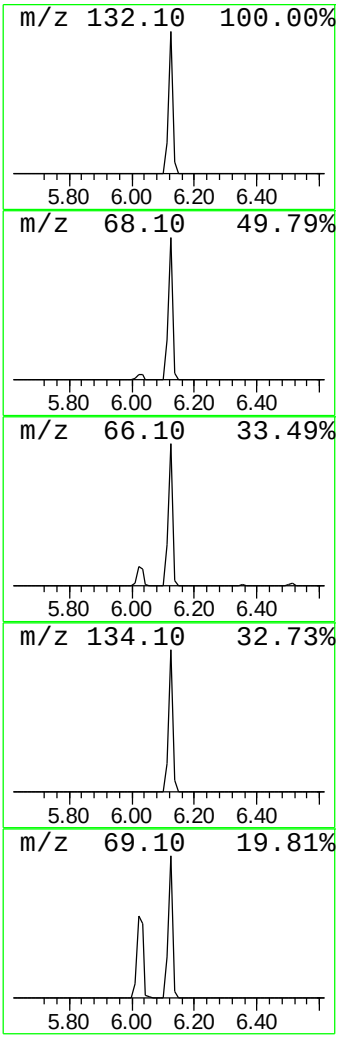
Peak Number 2 unknown6.12 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.12	101.68 ng	1754320	1,4-Dichlorobenzene-d4	6.35

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	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
5	1,2,3-Trifluorobenzene	132	C6H3F3	001489-53-8	9





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Sample : G3555-06
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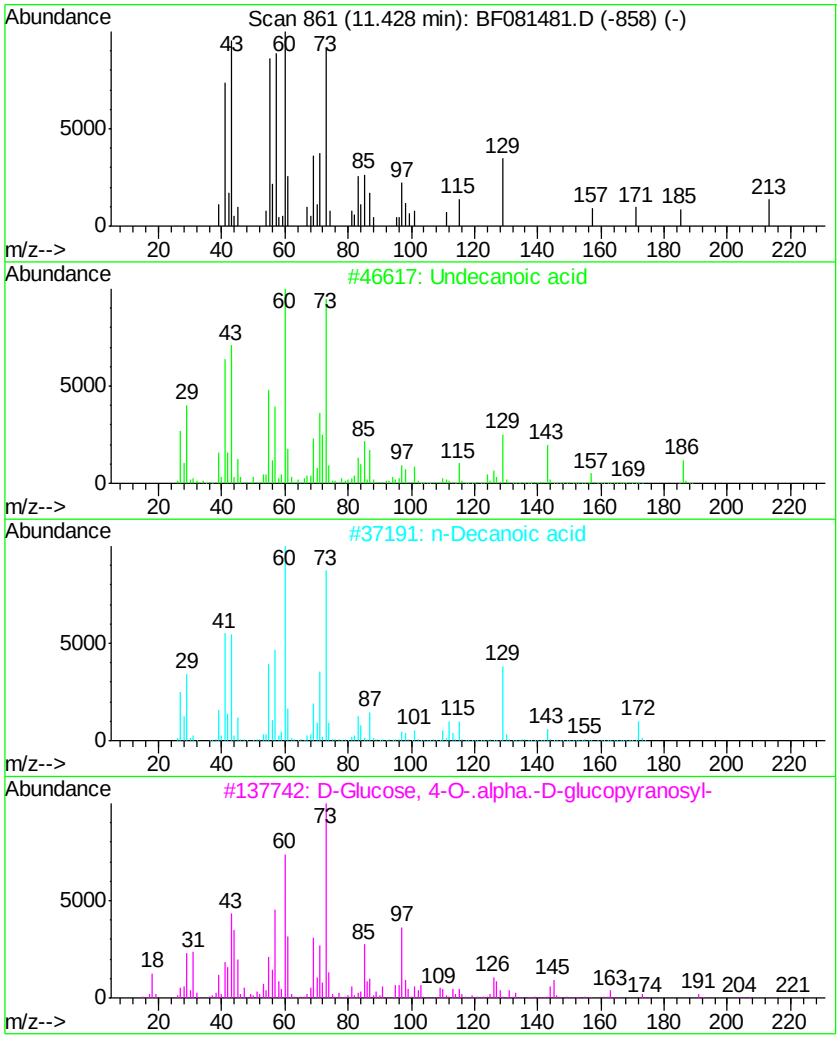
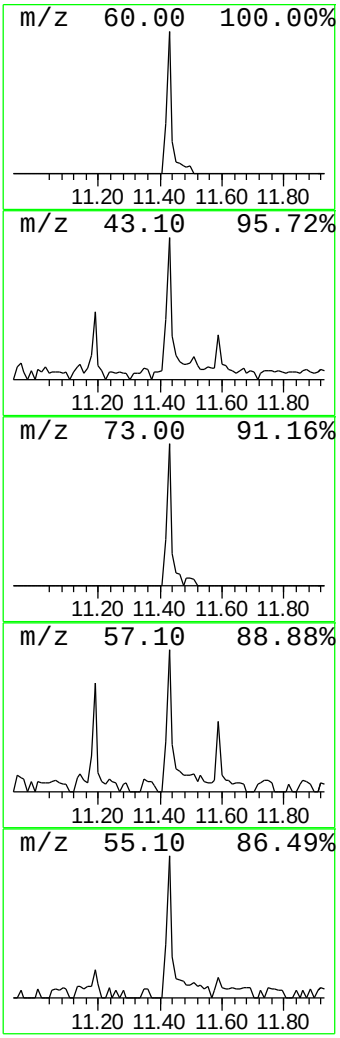
Peak Number 4 Undecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.43	3.63 ng	81969	Phenanthrene-d10	10.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecanoic acid	186	C11H22O2	000112-37-8	72
2	n-Decanoic acid	172	C10H20O2	000334-48-5	47
3	D-Glucose, 4-O-.alpha.-D-glucopy...	342	C12H22O11	000069-79-4	47
4	Dodecanoic acid	200	C12H24O2	000143-07-7	45
5	Nonanoic acid	158	C9H18O2	000112-05-0	43





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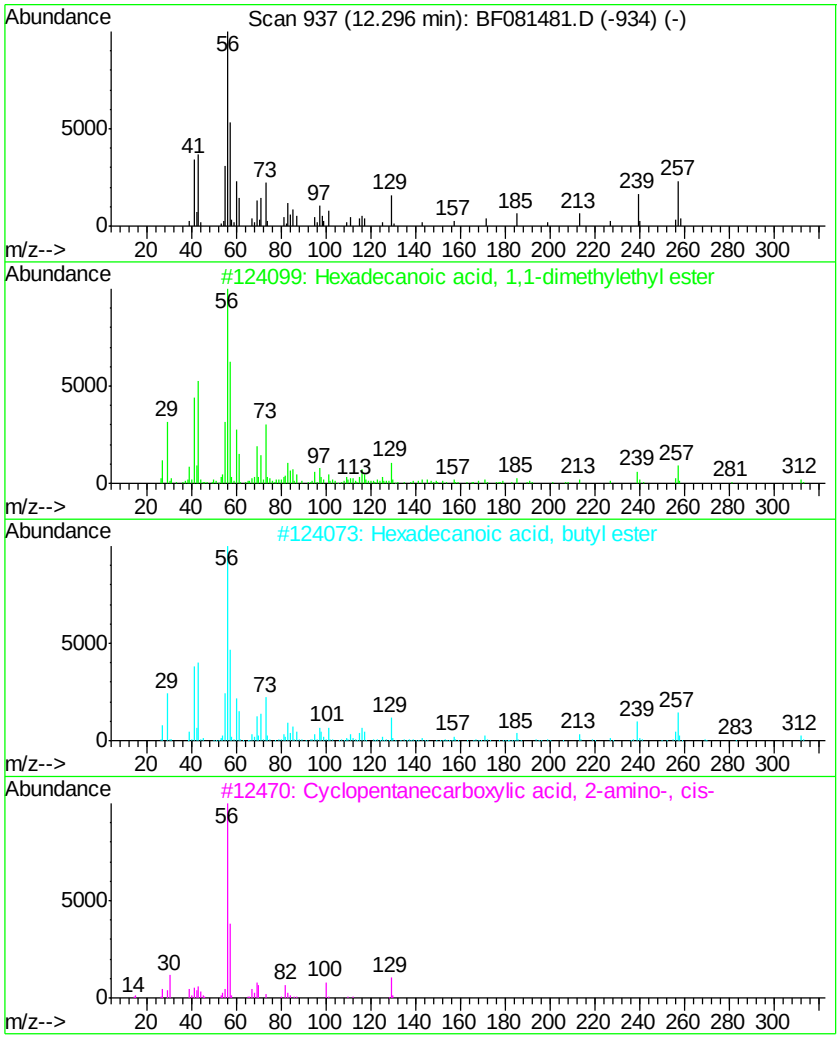
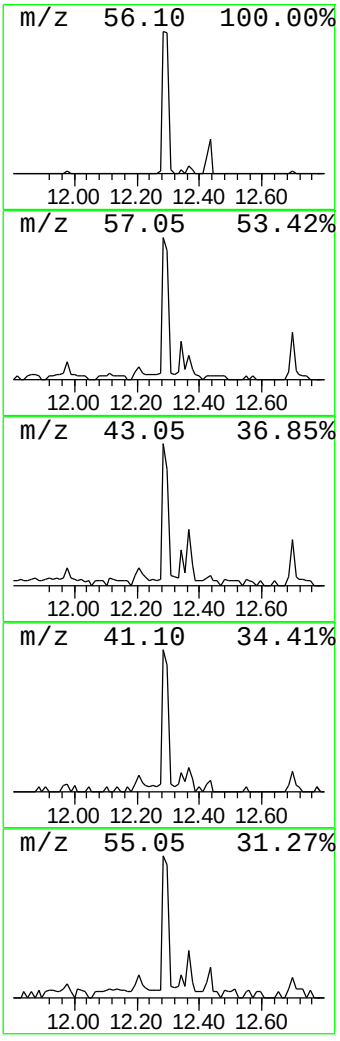
Peak Number 5 Hexadecanoic acid, 1,1-dime... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.30	9.32 ng	150216	Chrysene-d12	13.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	87
2	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	83
3	Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	037910-65-9	38
4	Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	35
5	2,4-Dipropyl-5-ethyl-1,3-dioxane	200	C12H24O2	006413-83-8	32





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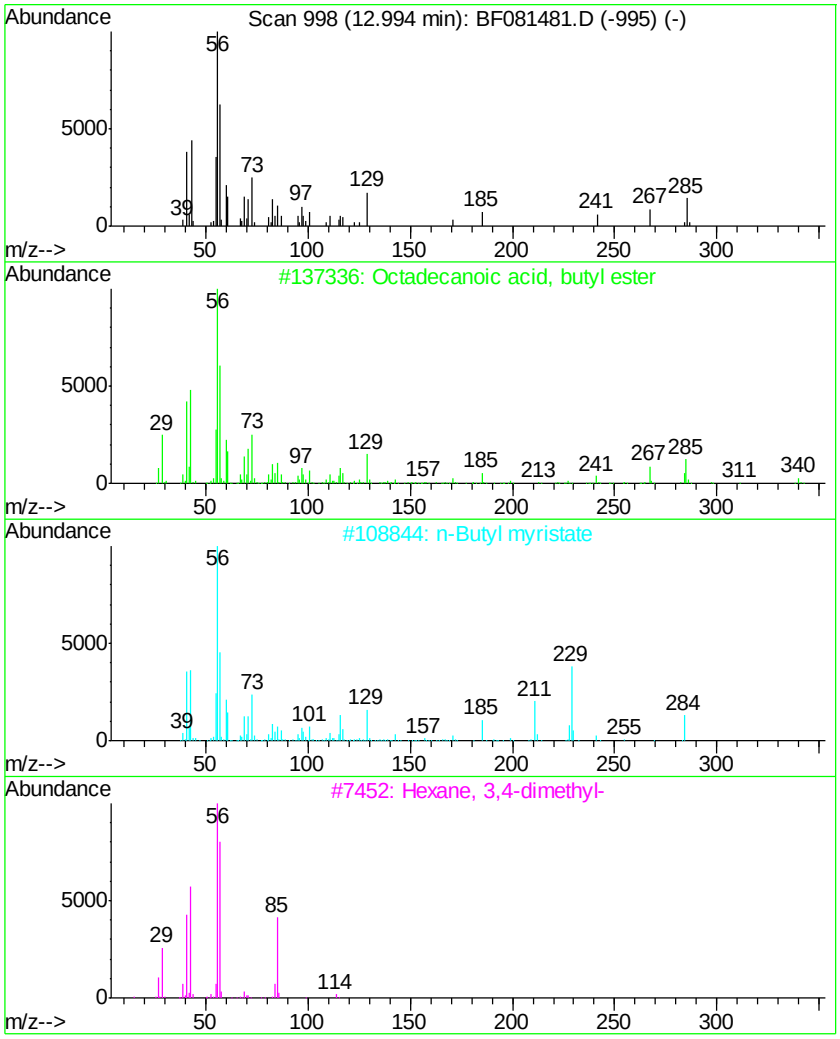
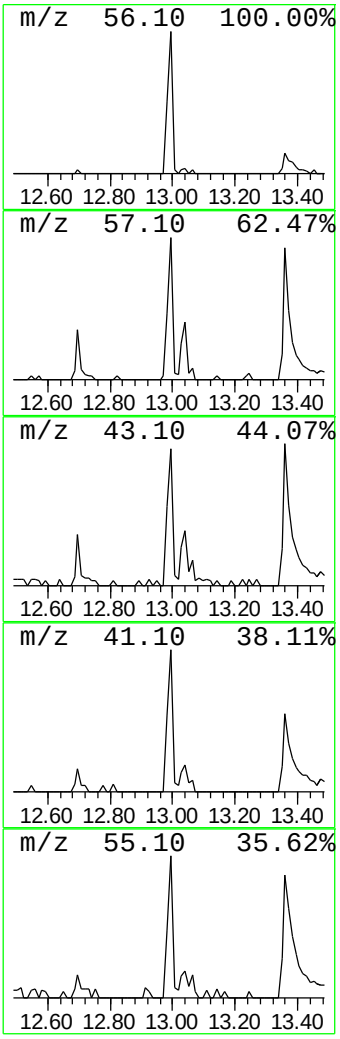
Peak Number 6 Octadecanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.99	6.53 ng	105222	Chrysene-d12	13.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	91
2	n-Butyl myristate	284	C18H36O2	000110-36-1	78
3	Hexane, 3,4-dimethyl-	114	C8H18	000583-48-2	38
4	Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	38
5	Pentadecane, 8-methylene-	224	C16H32	055668-09-2	37





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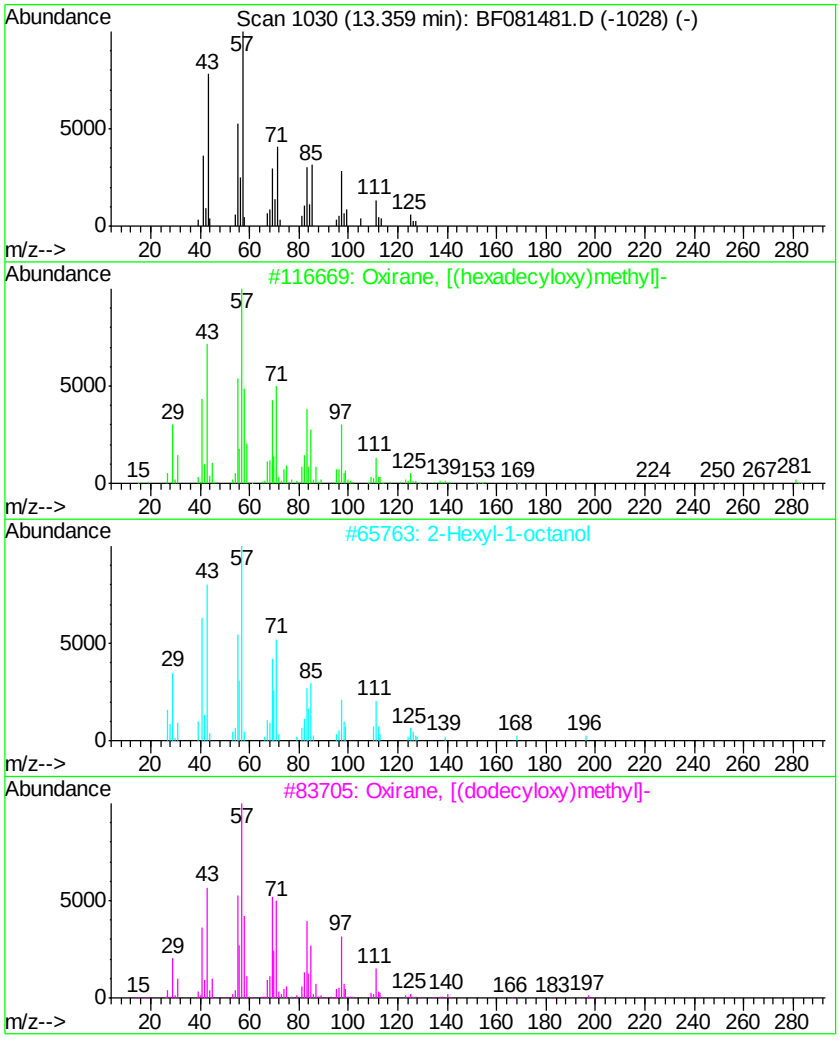
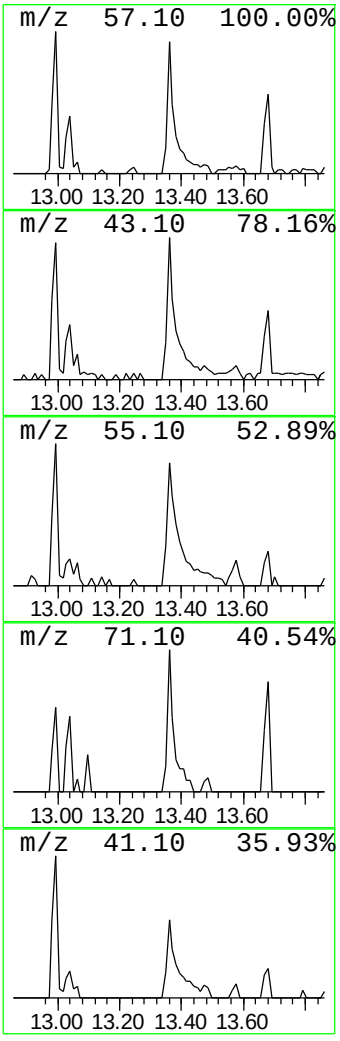
Peak Number 7 Oxirane, [(hexadecyloxy)met... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.36	8.16 ng	131540	Chrysene-d12	13.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, [(hexadecyloxy)methyl]-	298	C19H38O2	015965-99-8	80
2	2-Hexyl-1-octanol	214	C14H30O	019780-79-1	64
3	Oxirane, [(dodecyloxy)methyl]-	242	C15H30O2	002461-18-9	53
4	1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	50
5	Pentadecane	212	C15H32	000629-62-9	43





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
2-Pentanone, 4-hy...	4.41	72.5	ng	1251330	1	6.35	345065	20.0
unknown6.12	6.12	101.7	ng	1754320	1	6.35	345065	20.0
Undecanoic acid	11.43	3.6	ng	81969	4	10.84	451619	20.0
Hexadecanoic acid...	12.30	9.3	ng	150216	5	13.45	322275	20.0
Octadecanoic acid...	12.99	6.5	ng	105222	5	13.45	322275	20.0
Oxirane, [(hexade...	13.36	8.2	ng	131540	5	13.45	322275	20.0