LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF073115\
Data File : BF080735.D
Acq On : 31 Jul 2015 15:39
Operator : TP/UM
Sample : PB84765BL
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB84765BL

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-BF073015.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	2.213	7	11	15	rBV	18408	55507	1.28%	0.136%
2	4.407	201	203	209	rVB	324436	377227	8.72%	0.926%
3	5.059	256	260	273	rBV	2509722	3579732	82.72%	8.785%
4	5.459	292	295	298	rBV	3413373	3864589	89.30%	9.485%
5	5.870	329	331	333	rVB	100847	137703	3.18%	0.338%
6	6.476	381	384	387	rBV	3088372	3820468	88.28%	9.376%
7	6.624	394	397	399	rBV	3101620	4209203	97.26%	10.330%
8	6.853	415	417	419	rBV	1217496	1048877	24.24%	2.574%
9	7.013	428	431	433	rBV	2416304	3143822	72.65%	7.716%
10	7.413	463	466	468	rBV	2821987	2820395	65.17%	6.922%
11	8.133	526	529	531	rBV	1454946	1349497	31.18%	3.312%
12	9.208	620	623	626	rBV	3792758	4327586	100.00%	10.621%
13	9.882	679	682	685	rBV	1297328	1400927	32.37%	3.438%
14	10.671	748	751	753	rBV	2833600	2805592	64.83%	6.886%
15	11.368	809	812	814	rBV	1519334	1499475	34.65%	3.680%
16	12.774	933	935	938	rBV	108776	148749	3.44%	0.365%
17	12.956	948	951	953	rBV	3676775	4251917	98.25%	10.435%
18	13.482	995	997	999	rBV	130095	106780	2.47%	0.262%
19	13.528	999	1001	1002	rBV	55867	45828	1.06%	0.112%
20	13.997	1039	1042	1044	rBV	854759	971990	22.46%	2.385%
21	15.414	1163	1166	1169	rBV	571183	780291	18.03%	1.915%

Sum of corrected areas: 40746155

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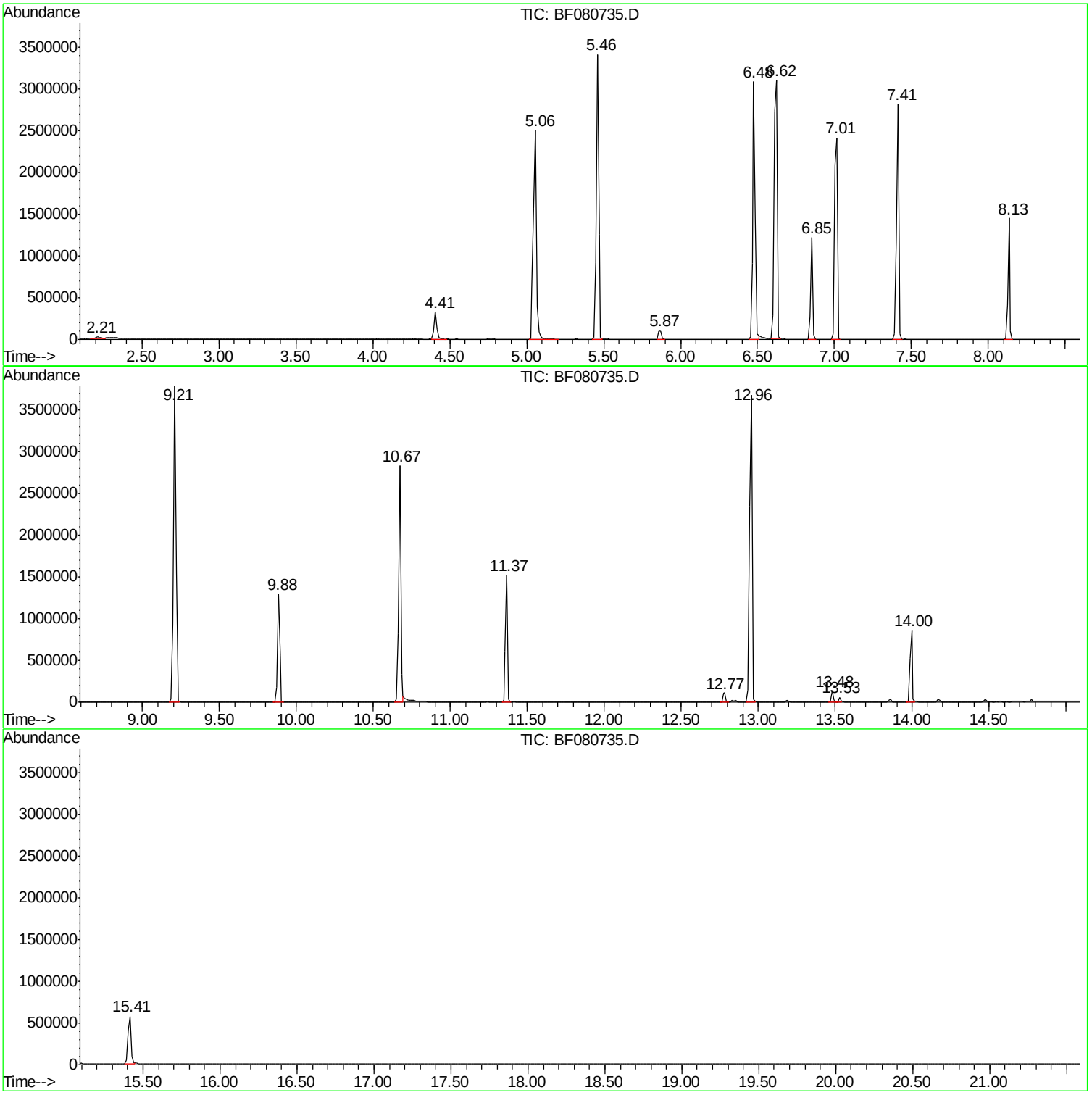
BNA_F
ClientSampleId :
PB84765BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF073015.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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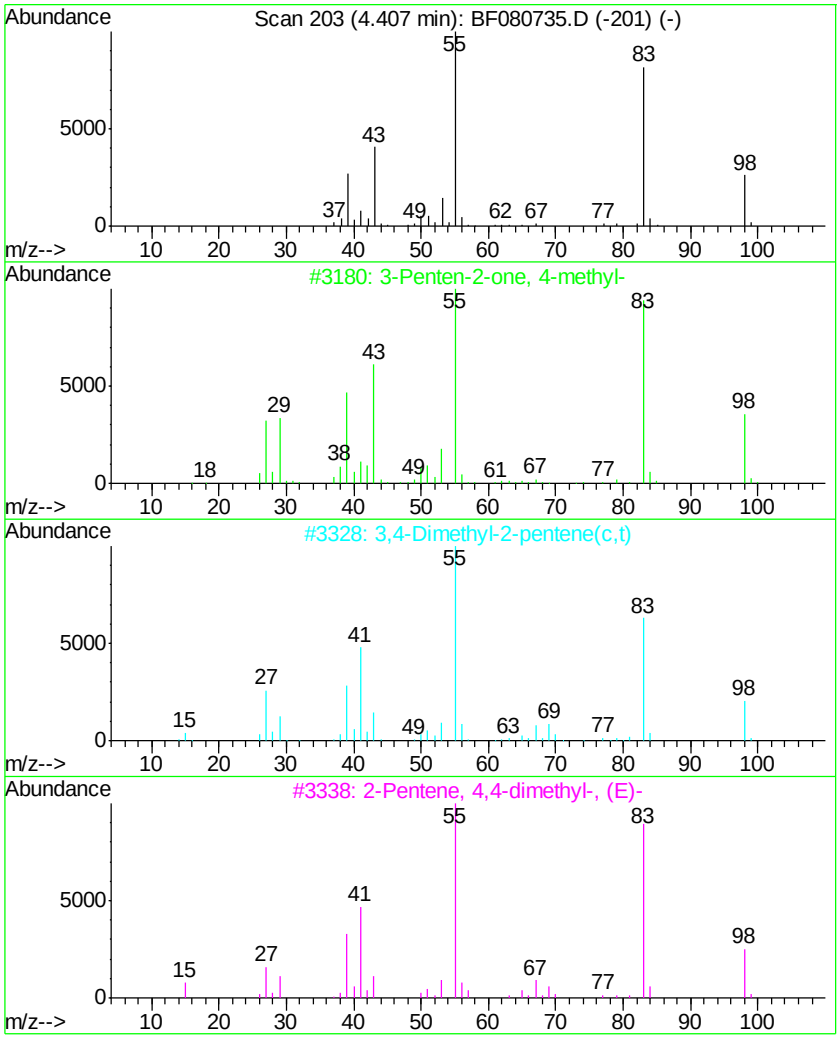
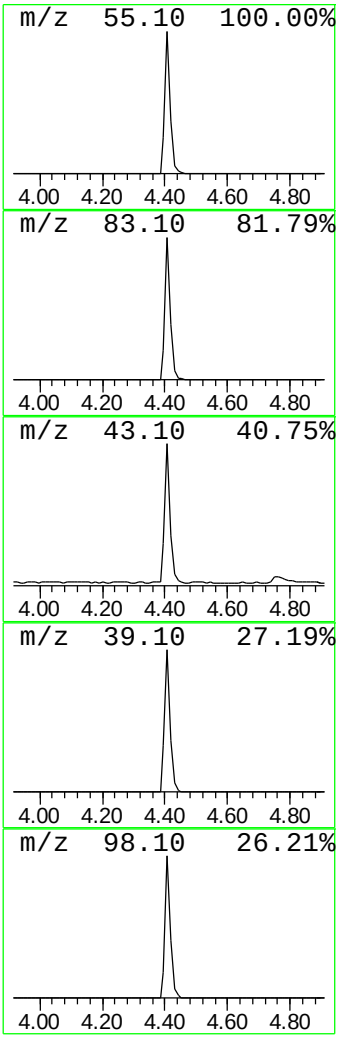
Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.41	7.19 ng	377227	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	93
2	3,4-Dimethyl-2-pentene(c,t)	98	C7H14	1000118-16-5	86
3	2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	78
4	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	78
5	3-Hexen-2-one	98	C6H10O	000763-93-9	72





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Instrument : BNA_F
ClientSampleId : PB84765BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF073015.M
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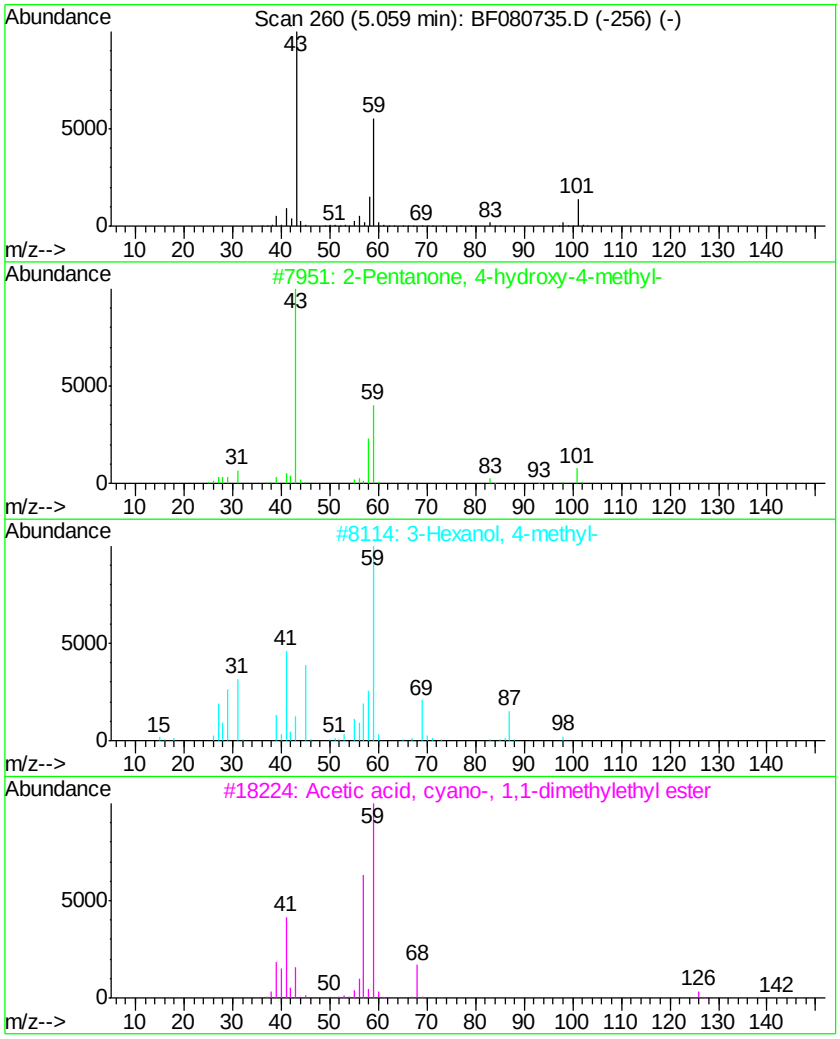
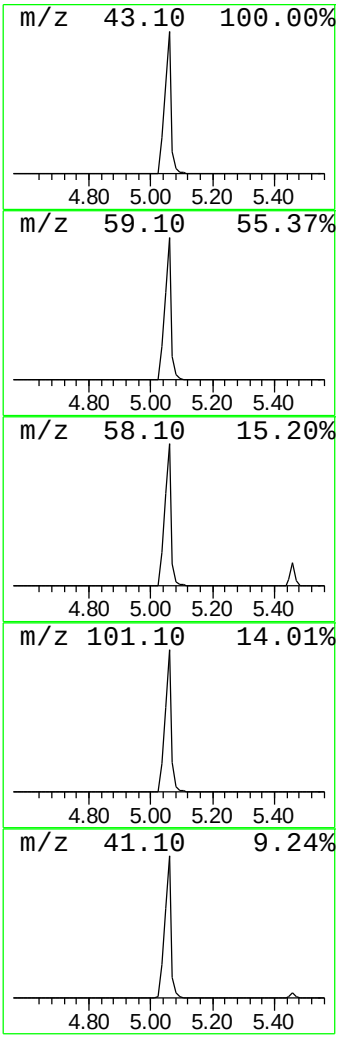
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.06	68.26 ng	3579730	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	23
5	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9





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Sample : PB84765BL
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB84765BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF073015.M
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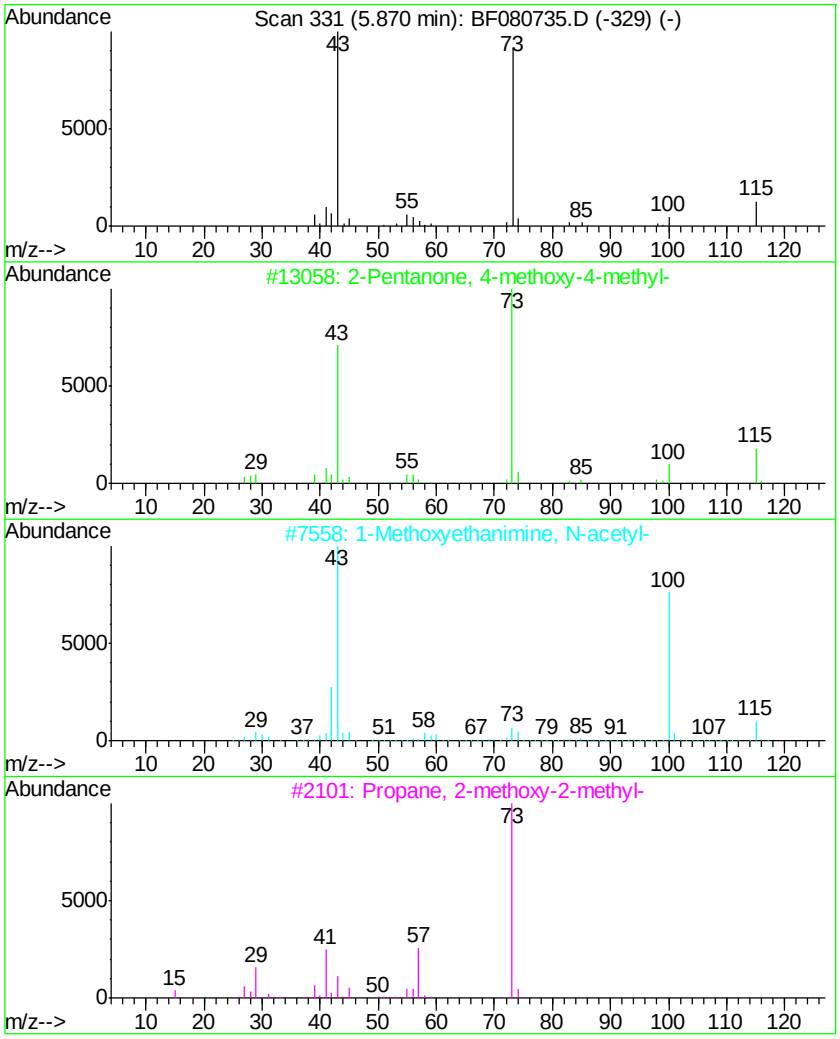
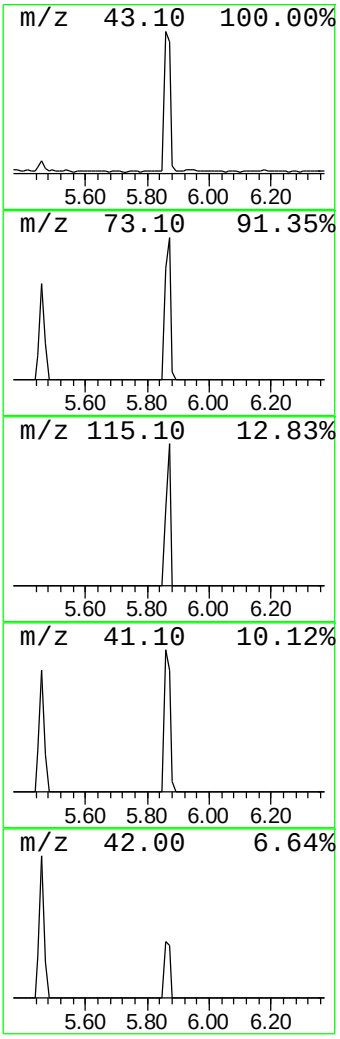
Peak Number 3 unknown5.87 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.87	2.63 ng	137703	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2	1-Methoxyethanimine, N-acetyl-	115	C5H9NO2	099028-43-0	28
3	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	12
4	2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	9
5	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9





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ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF073015.M
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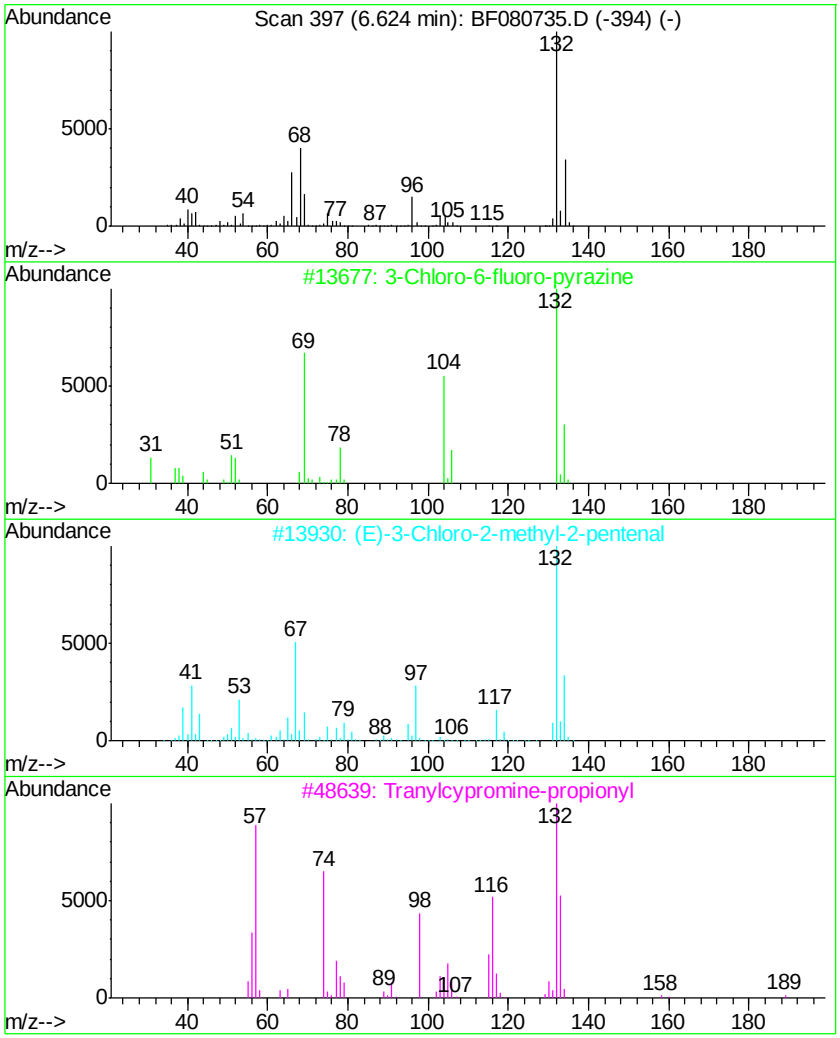
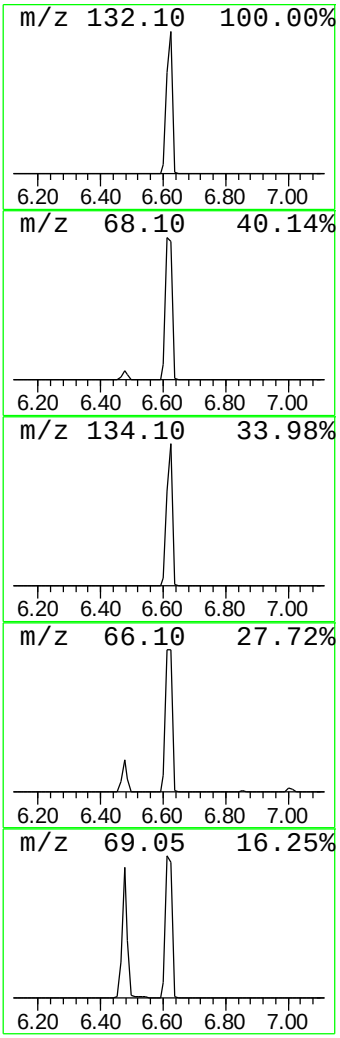
Peak Number 4 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	80.26 ng	4209200	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9
5	Benzene, 1,2,4-trifluoro-	132	C6H3F3	000367-23-7	9





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ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF073015.M
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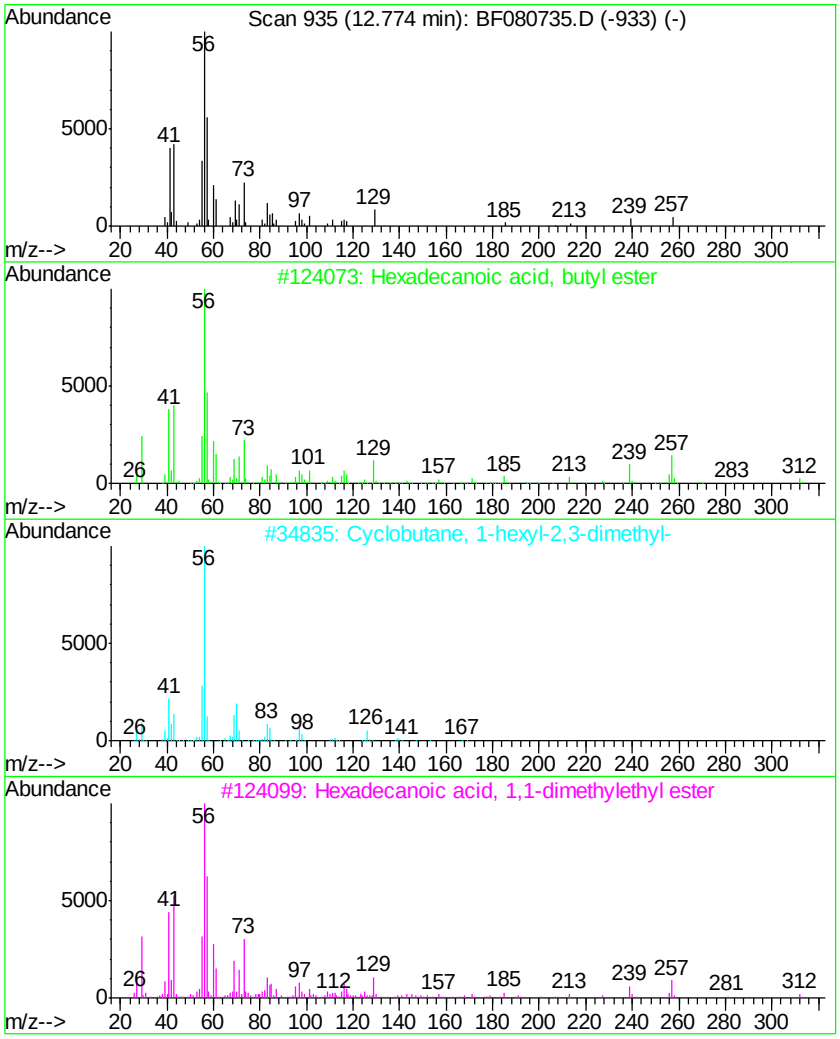
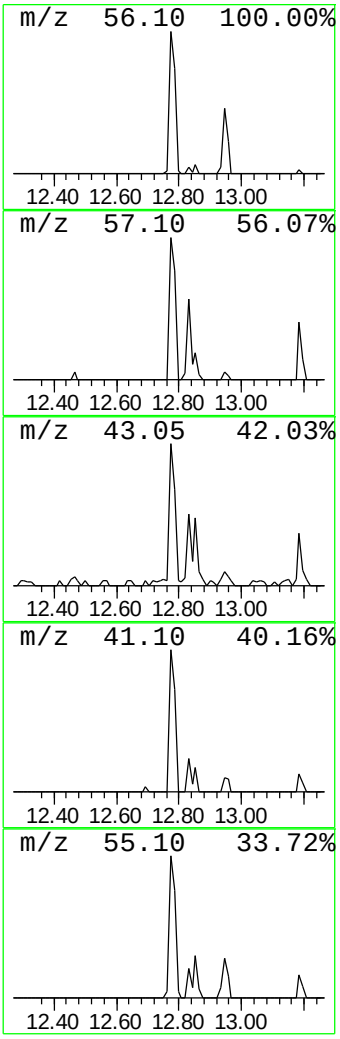
Peak Number 6 unknown12.77 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.77	3.06 ng	148749	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	47
2	Cyclobutane, 1-hexyl-2,3-dimethyl-	168	C12H24	055170-84-8	43
3	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	43
4	1-Pentene, 2,4-dimethyl-	98	C7H14	002213-32-3	38
5	1-Undecene, 2-methyl-	168	C12H24	018516-37-5	38





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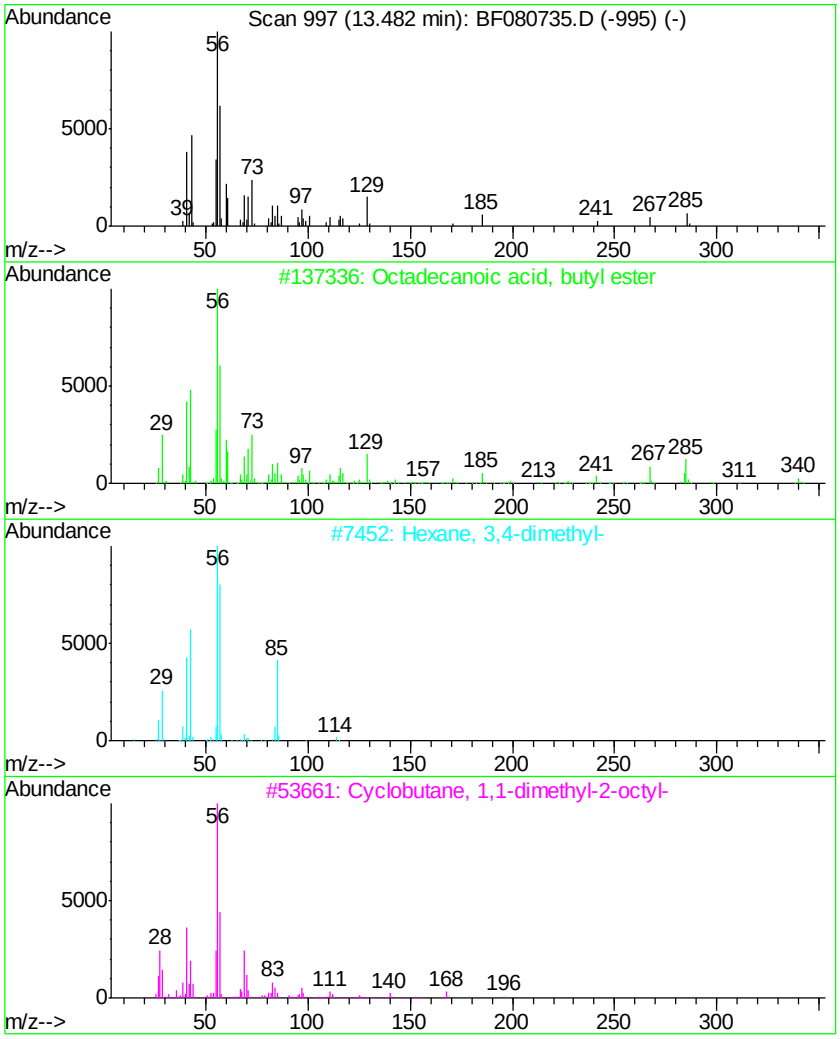
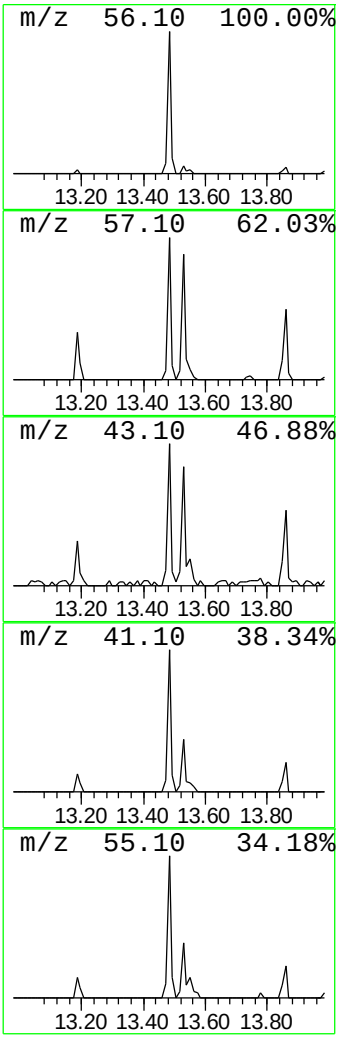
Peak Number 7 Octadecanoic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.48	2.20 ng	106780	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	91
2	Hexane, 3,4-dimethyl-	114	C8H18	000583-48-2	38
3	Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	38
4	Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	040482-05-1	37
5	1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	35





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
3-Penten-2-one, 4...	4.41	7.2	ng	377227	1	6.85	1048880	20.0
2-Pentanone, 4-hy...	5.06	68.3	ng	3579730	1	6.85	1048880	20.0
unknown5.87	5.87	2.6	ng	137703	1	6.85	1048880	20.0
unknown6.62	6.62	80.3	ng	4209200	1	6.85	1048880	20.0
unknown12.77	12.77	3.1	ng	148749	5	14.00	971990	20.0
Octadecanoic acid...	13.48	2.2	ng	106780	5	14.00	971990	20.0