LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF073115\
Data File : BF080756.D
Acq On : 1 Aug 2015 2:34
Operator : TP/UM
Sample : G3127-09
Misc :
ALS Vial : 48 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COFF-3RD-8(0-2)

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	2.155	4	6	9	rBV	38533	49805	1.35%	0.154%
2	4.396	200	202	207	rVB	109189	132972	3.61%	0.412%
3	5.047	255	259	262	rBV	1992434	3122503	84.88%	9.674%
4	5.458	292	295	297	rBV	3501583	3678665	100.00%	11.397%
5	5.859	328	330	333	rVB	124837	126396	3.44%	0.392%
6	6.476	381	384	387	rBV	3005658	3309497	89.96%	10.253%
7	6.613	394	396	399	rBV	2608389	3368937	91.58%	10.437%
8	6.853	414	417	419	rBB	941860	821682	22.34%	2.546%
9	7.002	428	430	433	rBV	1700993	2212802	60.15%	6.856%
10	7.413	463	466	468	rBV	2426297	2405520	65.39%	7.453%
11	8.133	526	529	531	rBV	1177018	1025588	27.88%	3.177%
12	9.207	620	623	626	rBV	3248219	3022948	82.18%	9.365%
13	9.607	655	658	660	rBV	564830	641506	17.44%	1.987%
14	9.882	680	682	685	rBV	1061573	1009895	27.45%	3.129%
15	10.316	719	720	722	rVB	32556	44262	1.20%	0.137%
16	10.670	748	751	753	rBV	2005580	2050076	55.73%	6.351%
17	10.796	760	762	765	rBV	80499	91706	2.49%	0.284%
18	11.242	799	801	802	rBV	77911	64895	1.76%	0.201%
19	11.368	809	812	814	rBV	925059	995026	27.05%	3.083%
20	11.665	836	838	845	rVB	52920	53169	1.45%	0.165%
21	11.893	856	858	863	rVB	83932	97089	2.64%	0.301%
22	12.156	878	881	883	rVB	82393	91609	2.49%	0.284%
23	12.945	948	950	953	rBV	2500800	2516123	68.40%	7.795%
24	13.985	1039	1041	1044	rBV	529479	668456	18.17%	2.071%
25	14.111	1044	1052	1056	rVV6	14133	82786	2.25%	0.256%
26	15.402	1162	1165	1168	rBV	429664	593688	16.14%	1.839%

Sum of corrected areas: 32277601

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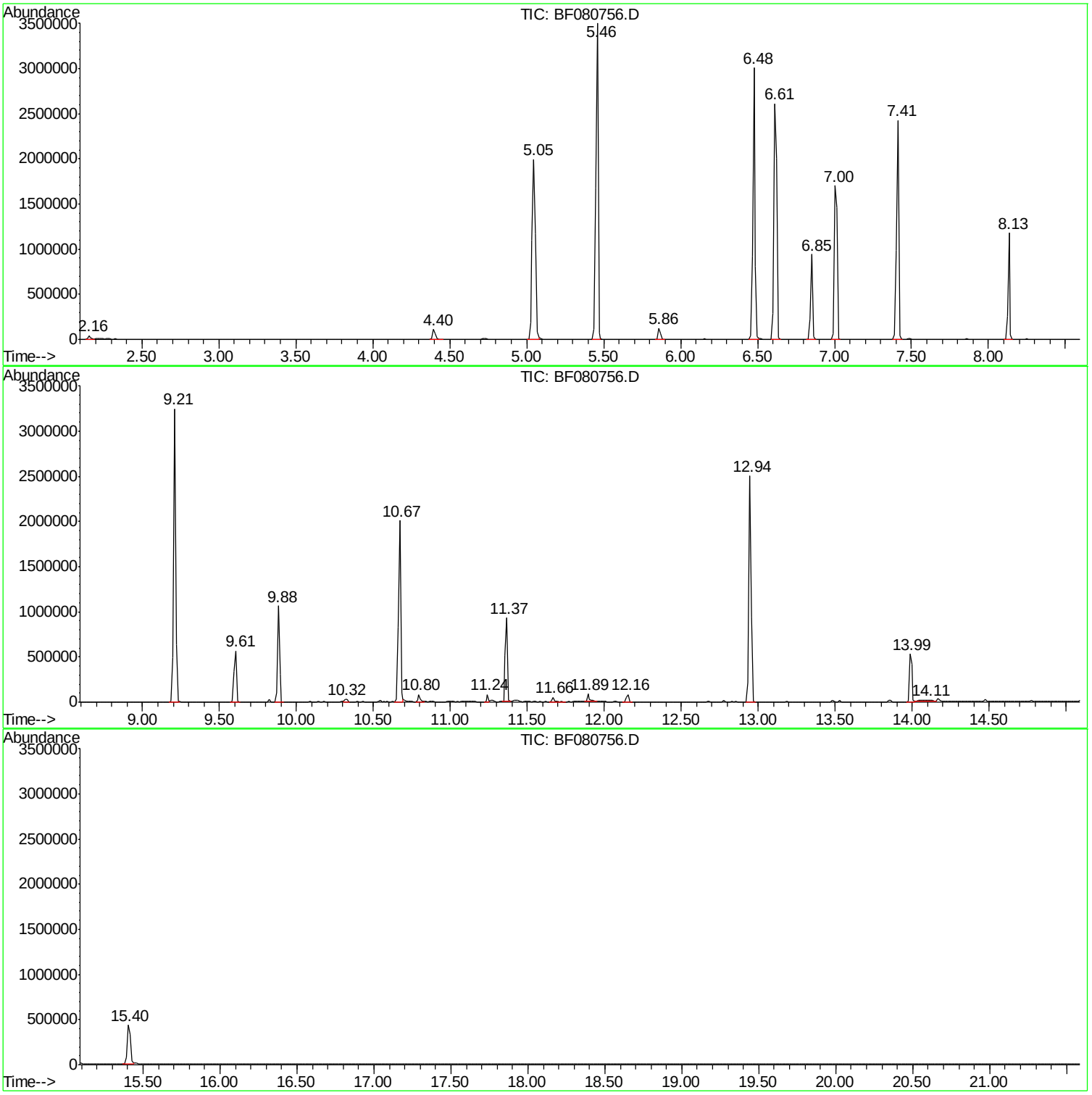
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF073015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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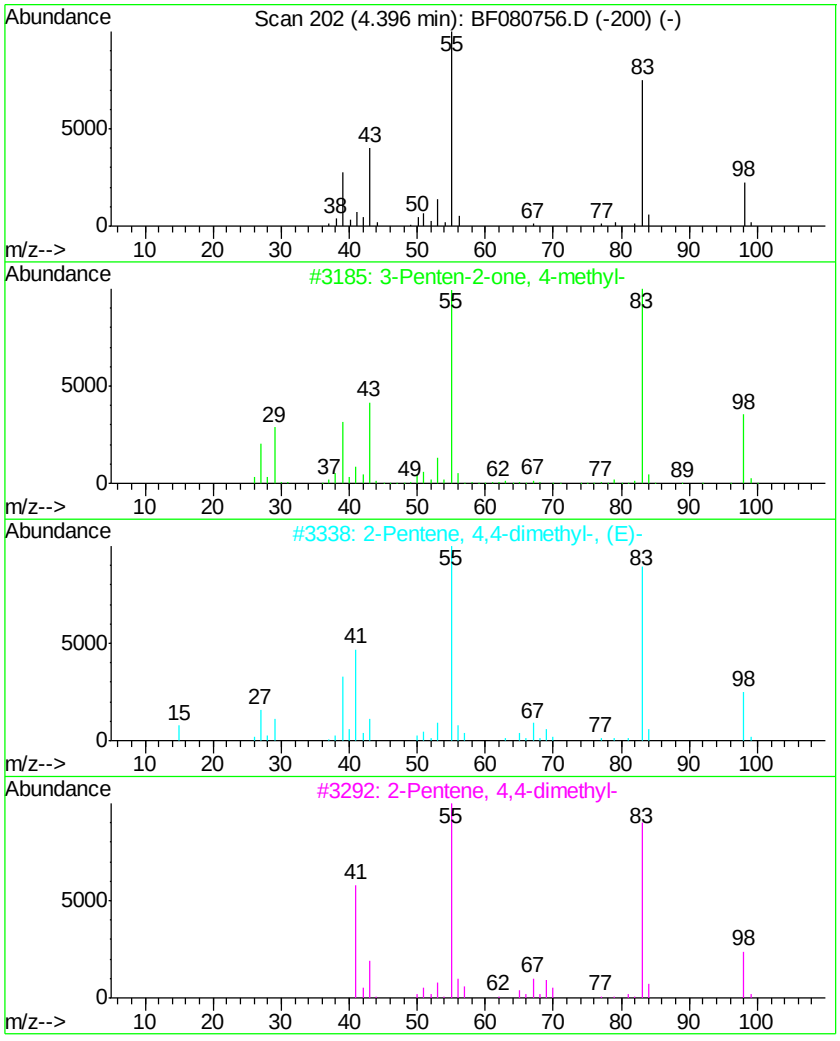
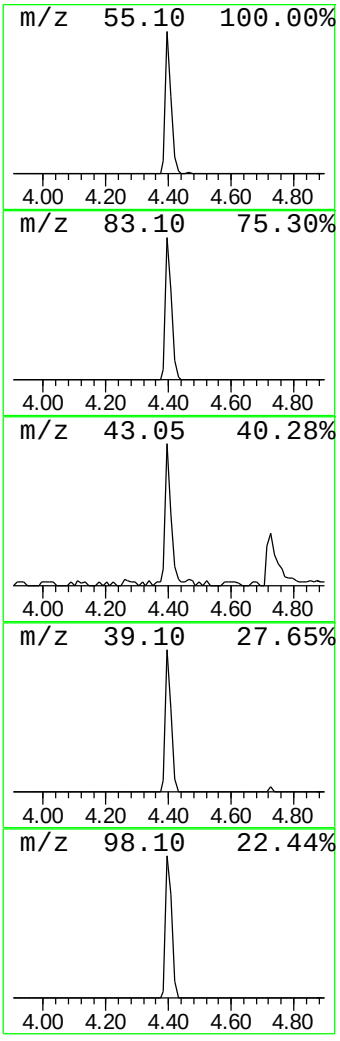
Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.40	3.24 ng	132972	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	90
2	2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	86
3	2-Pentene, 4,4-dimethyl-	98	C7H14	026232-98-4	86
4	3,4-Dimethyl-2-pentene(c,t)	98	C7H14	1000118-16-5	86
5	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	80





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ClientSampleId : COFF-3RD-8(0-2)

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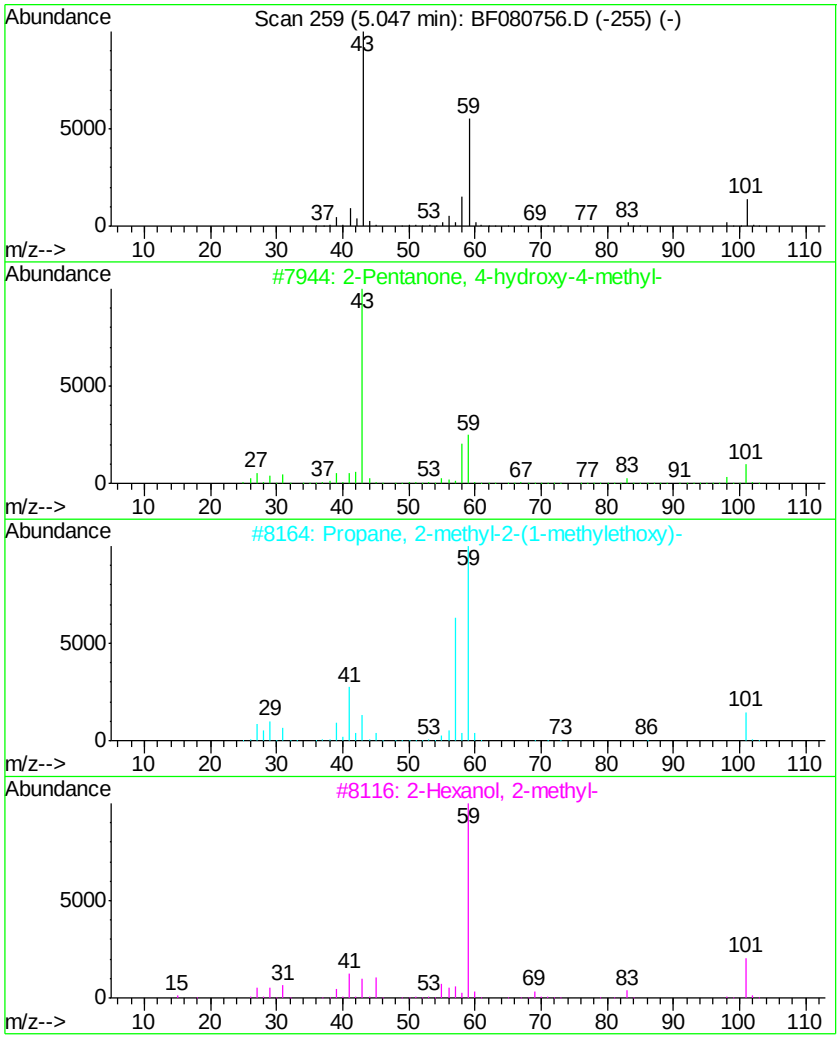
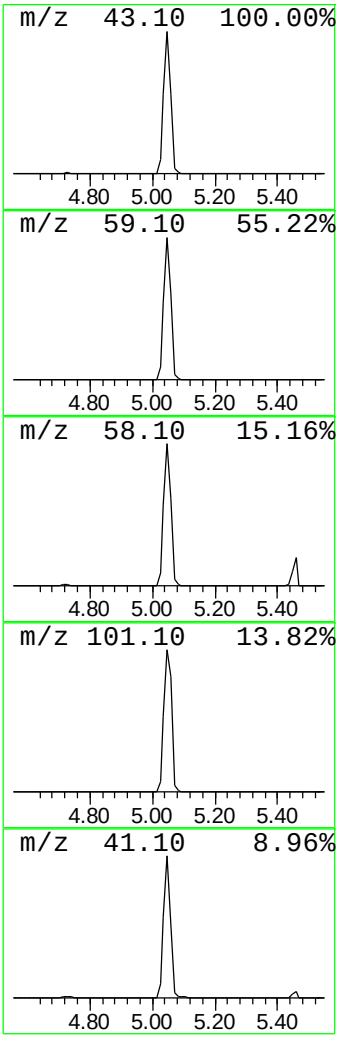
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.05	76.00 ng	3122500	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	59
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
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	32





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Instrument : BNA_F
ClientSampleId : COFF-3RD-8(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF073015.M
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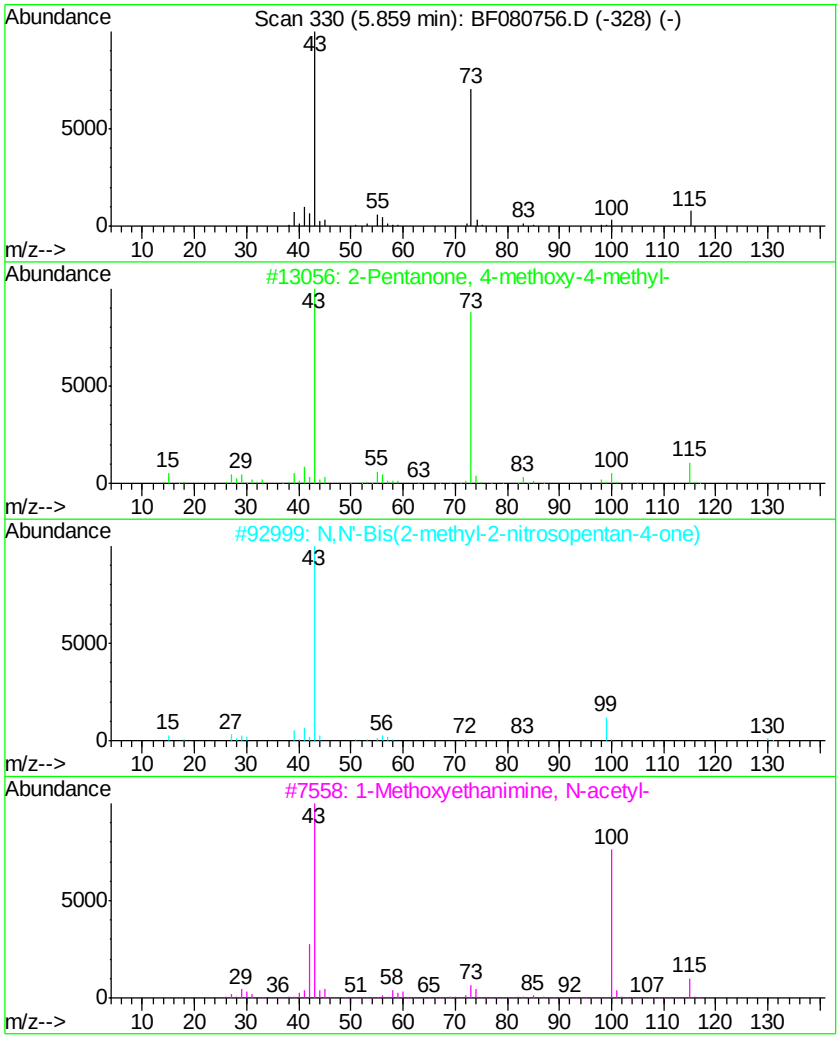
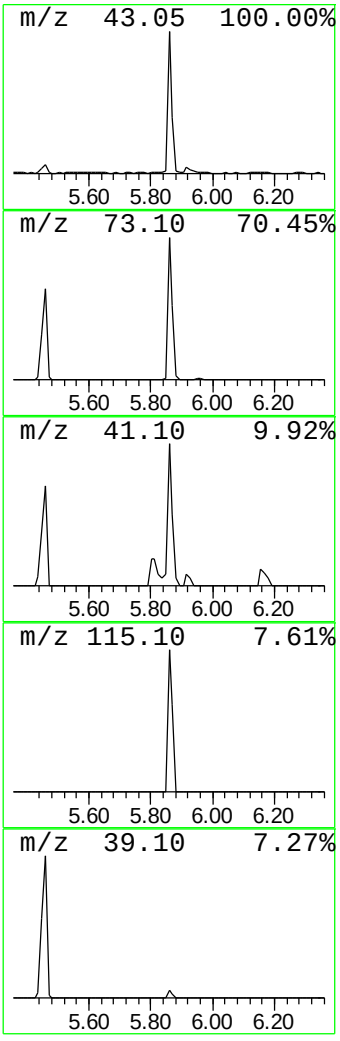
Peak Number 3 unknown5.86 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.86	3.08 ng	126396	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	78
2	N,N'-Bis(2-methyl-2-nitrosopenta...	258	C12H22N2O4	094514-30-4	25
3	1-Methoxyethanimine, N-acetyl-	115	C5H9NO2	099028-43-0	10
4	2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	9
5	Guanidine, methyl-	73	C2H7N3	000471-29-4	9





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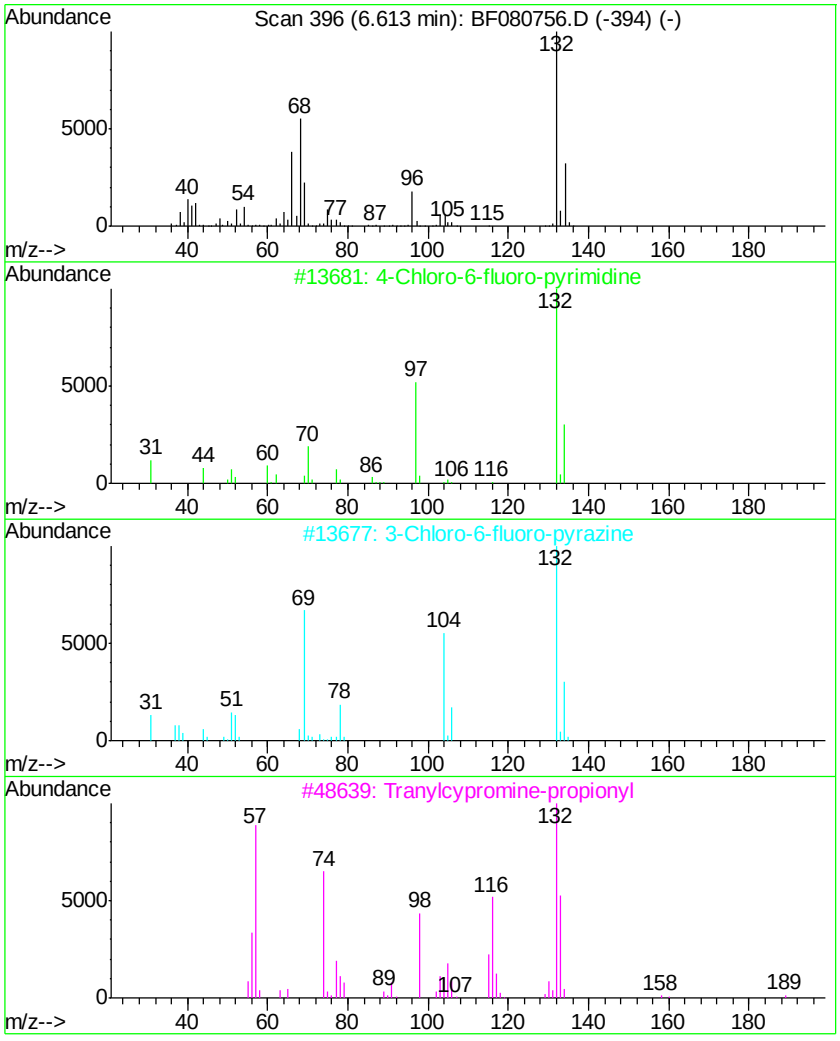
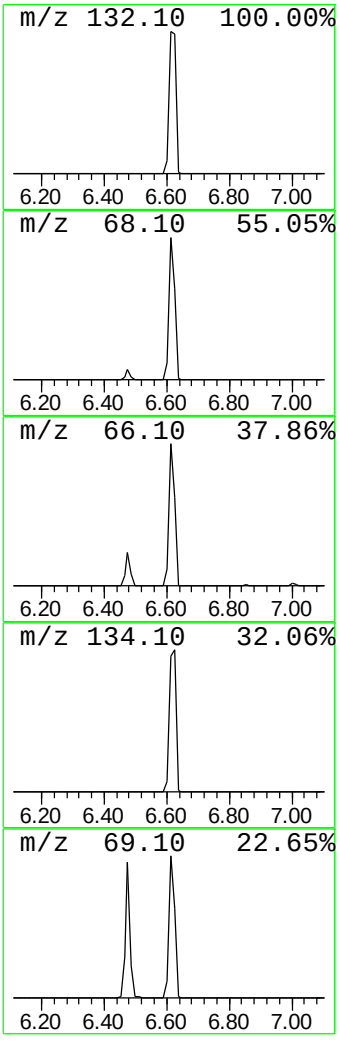
Peak Number 4 unknown6.61 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.61	82.00 ng	3368940	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	22
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12





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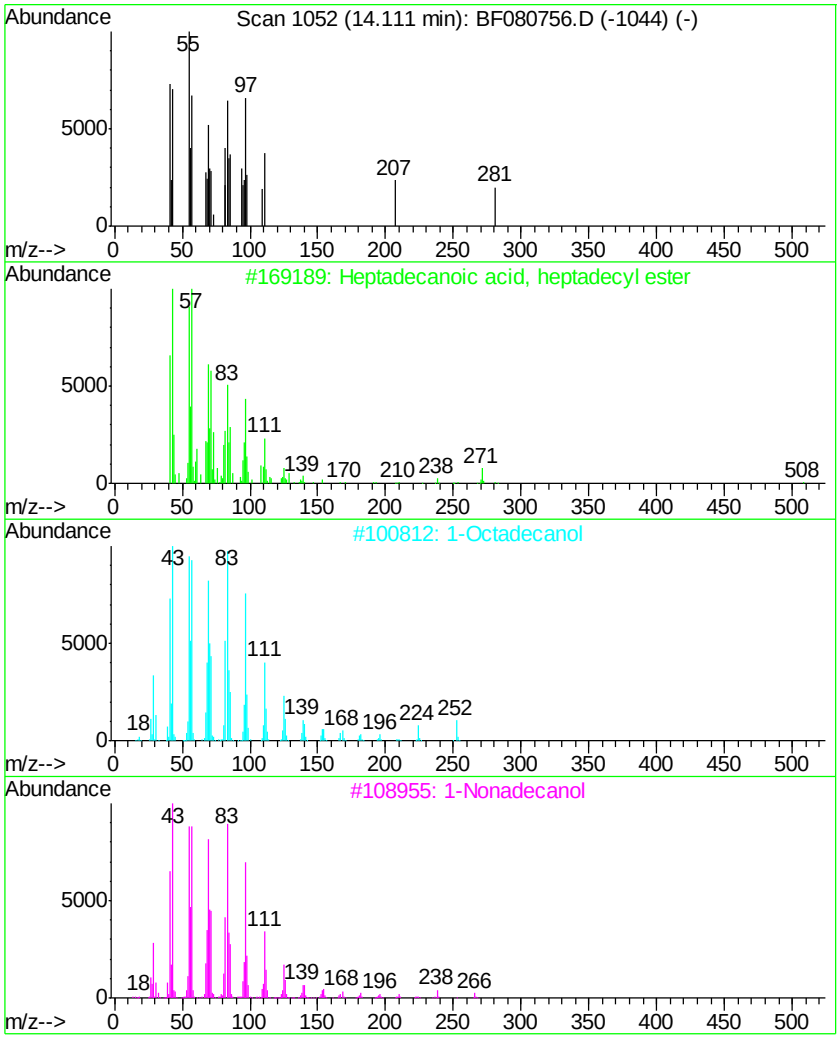
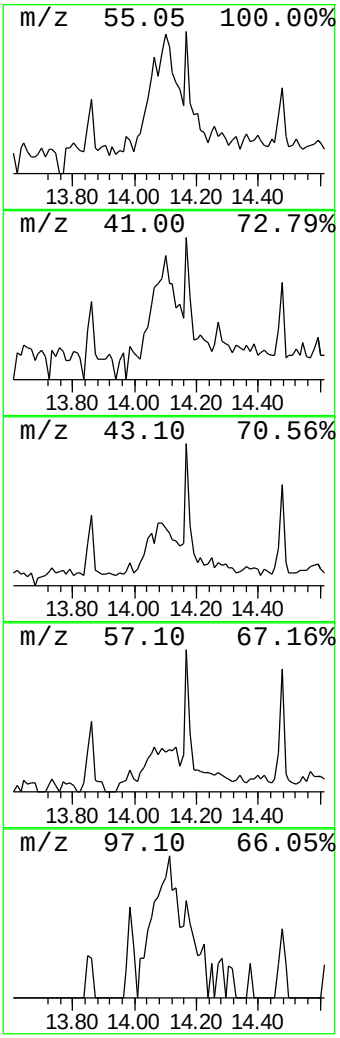
Peak Number 6 unknown14.11 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.11	2.48 ng	82786	Chrysene-d12	13.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecanoic acid, heptadecyl e...	509	C34H68O2	036617-50-2	47
2	1-Octadecanol	270	C18H38O	000112-92-5	43
3	1-Nonadecanol	284	C19H40O	001454-84-8	43
4	Acetic acid, chloro-, hexadecyl ...	318	C18H35ClO2	052132-58-8	43
5	1-Eicosanol	298	C20H42O	000629-96-9	43





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...	4.40	3.2	ng	132972	1	6.85	821682	20.0
2-Pentanone, 4-hy...	5.05	76.0	ng	3122500	1	6.85	821682	20.0
unknown5.86	5.86	3.1	ng	126396	1	6.85	821682	20.0
unknown6.61	6.61	82.0	ng	3368940	1	6.85	821682	20.0
unknown14.11	14.11	2.5	ng	82786	5	13.98	668456	20.0