LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM083117\
Data File : BM011388.D
Acq On : 01 Sep 2017 00:57
Operator : SJ/JU
Sample : I4963-09
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 3828-SPP4-DUP

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_M\METHODS\8270-BM083117.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	3.058	41	46	56	rBV	1184843	2160739	6.18%	1.285%
2	3.134	56	59	71	rVB	489865	659663	1.89%	0.392%
3	5.081	384	390	398	rBV	303074	456544	1.31%	0.271%
4	5.546	462	469	479	rBV	5125127	7499673	21.45%	4.459%
5	7.134	732	739	749	rBV	3124024	4878169	13.95%	2.900%
6	7.516	794	804	814	rBV	8731776	13803611	39.48%	8.206%
7	7.987	877	884	891	rBV	1821047	2984830	8.54%	1.775%
8	8.310	932	939	948	rBV	7277674	12046768	34.45%	7.162%
9	9.151	1074	1082	1092	rBV	6126042	10175268	29.10%	6.049%
10	10.798	1354	1362	1371	rVB	2655655	4442592	12.71%	2.641%
11	11.445	1466	1472	1484	rVB	347970	627298	1.79%	0.373%
12	13.245	1766	1778	1786	rBV	16427491	23913787	68.39%	14.217%
13	14.621	2004	2012	2021	rBV2	3895229	5779575	16.53%	3.436%
14	16.104	2256	2264	2274	rBV	12220874	17055917	48.78%	10.140%
15	17.357	2471	2477	2482	rBV	4730645	6821366	19.51%	4.055%
16	19.404	2821	2825	2832	rVB	315224	427476	1.22%	0.254%
17	19.768	2882	2887	2895	rVB	354311	495667	1.42%	0.295%
18	19.968	2915	2921	2929	rBV	27543799	34966809	100.00%	20.788%
19	20.721	3045	3049	3053	rBV	382094	423842	1.21%	0.252%
20	21.427	3166	3169	3175	rVB	480522	502675	1.44%	0.299%
21	21.521	3179	3185	3189	rVV	6983030	9088654	25.99%	5.403%
22	21.556	3189	3191	3196	rVB	453150	505070	1.44%	0.300%
23	22.344	3322	3325	3330	rVB	321074	419415	1.20%	0.249%
24	23.903	3583	3590	3601	rVB	4010945	8071109	23.08%	4.798%

Sum of corrected areas: 168206517

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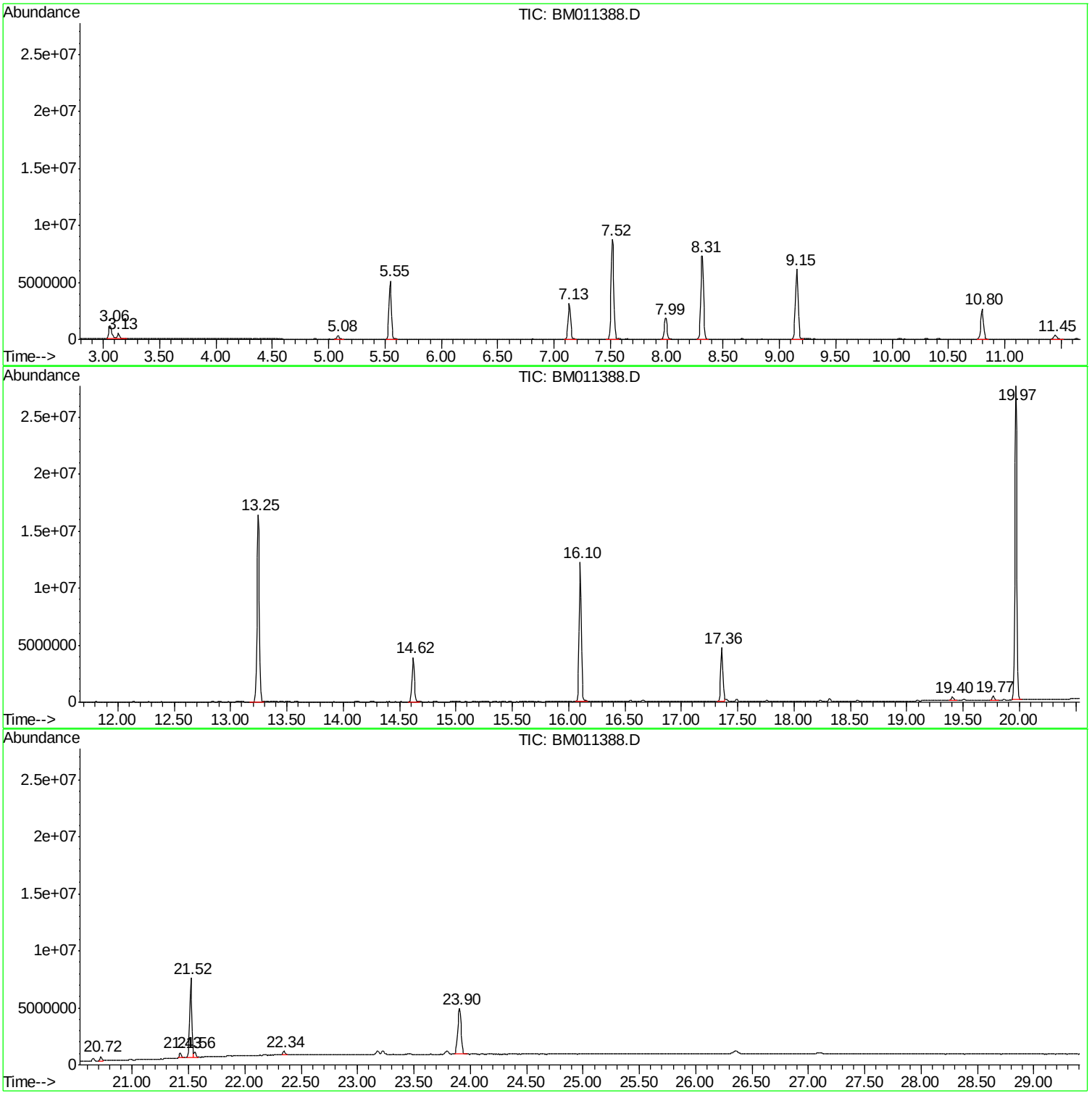
3828-SPP4-DUP

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM083117.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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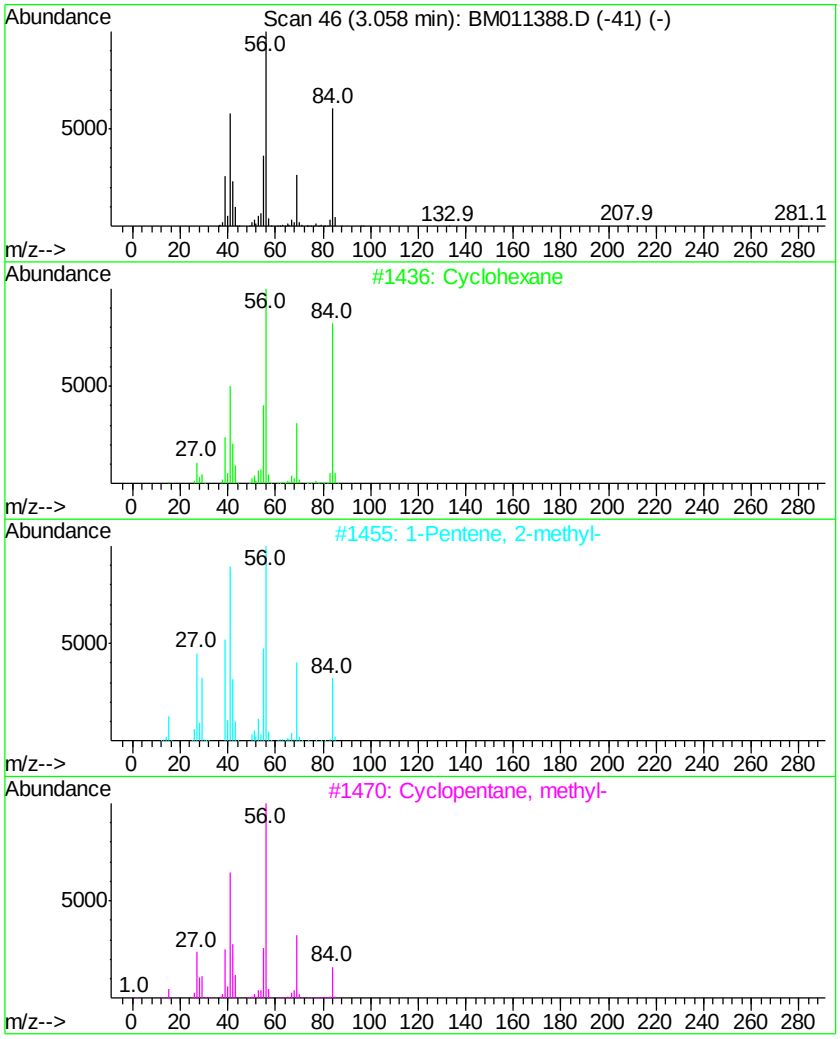
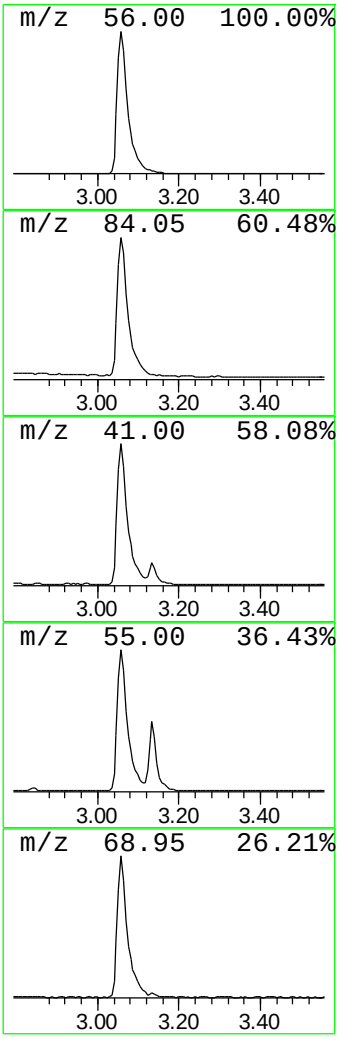
Peak Number 1 Cyclohexane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.06	14.48 ng	2160740	1,4-Dichlorobenzene-d4	7.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane	84	C6H12	000110-82-7	94
2	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	64
3	Cyclopentane, methyl-	84	C6H12	000096-37-7	59
4	Cyclobutane, ethyl-	84	C6H12	004806-61-5	50
5	1-Hexene, 5-methyl-	98	C7H14	003524-73-0	47





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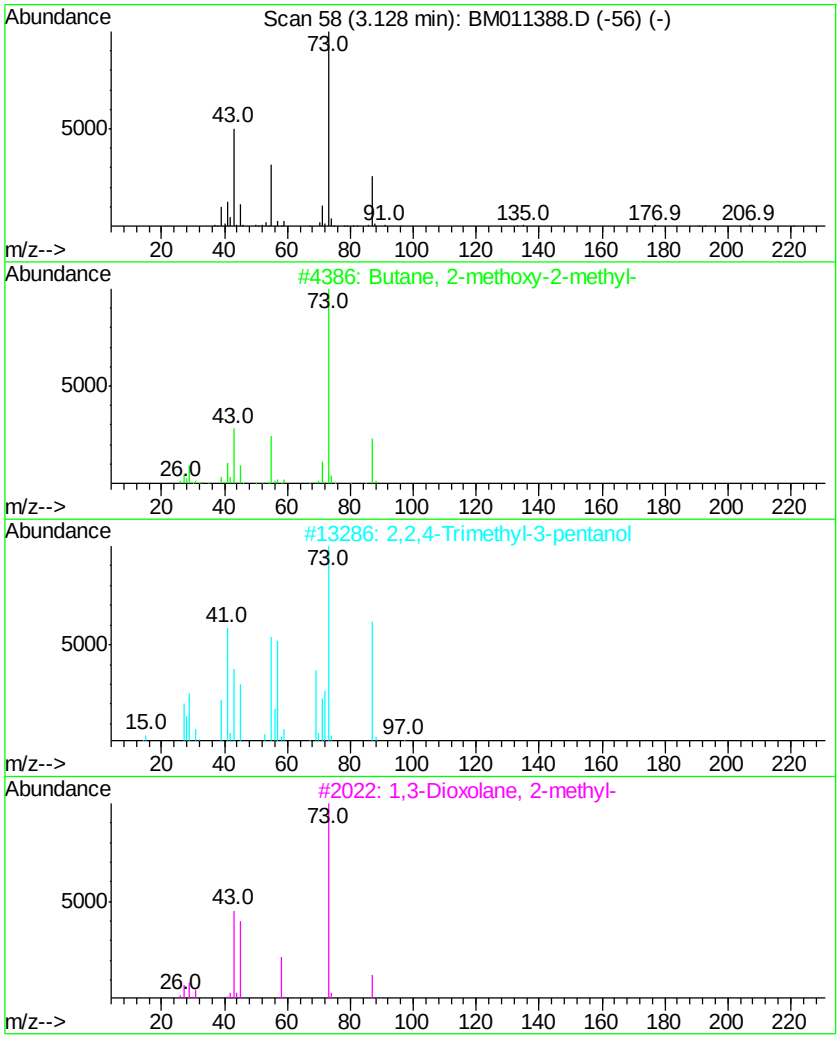
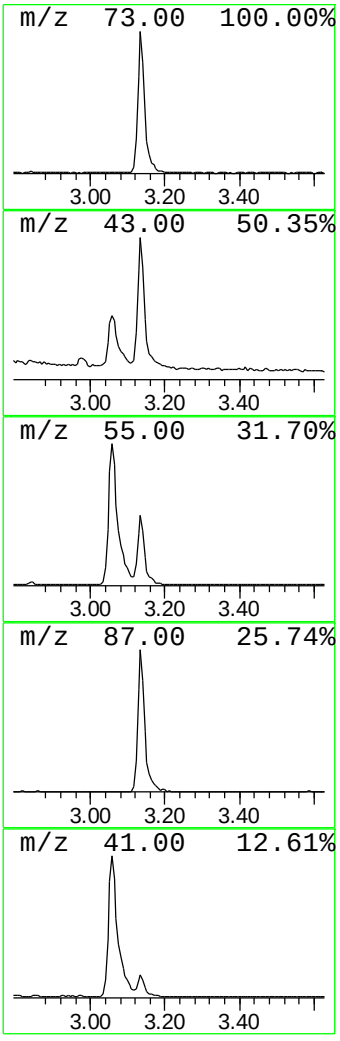
Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.13	4.42 ng	659663	1,4-Dichlorobenzene-d4	7.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	28
4	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9





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Instrument : BNA_M
ClientSampleId : 3828-SPP4-DUP

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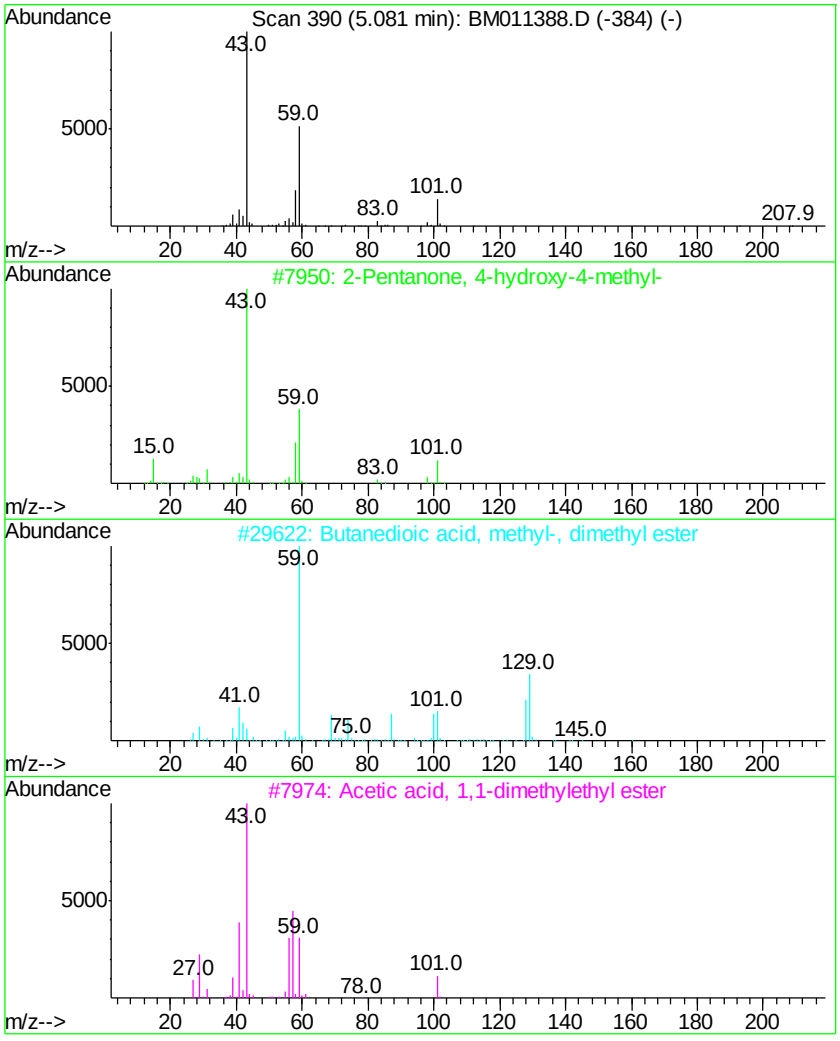
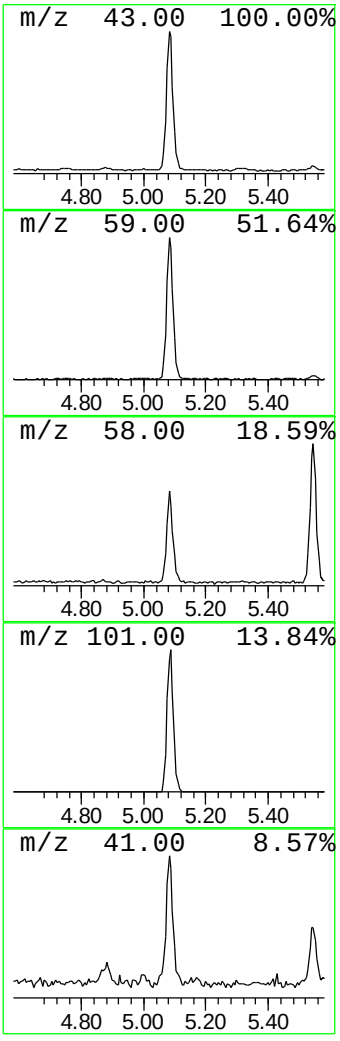
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.08	3.06 ng	456544	1,4-Dichlorobenzene-d4	7.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Butanedioic acid, methyl-, dimet...	160	C7H12O4	001604-11-1	28
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	Formamide, N,N-diethyl-	101	C5H11NO	000617-84-5	9





Library Search Compound Report

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Instrument : BNA_M
ClientSampleId : 3828-SPP4-DUP

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM083117.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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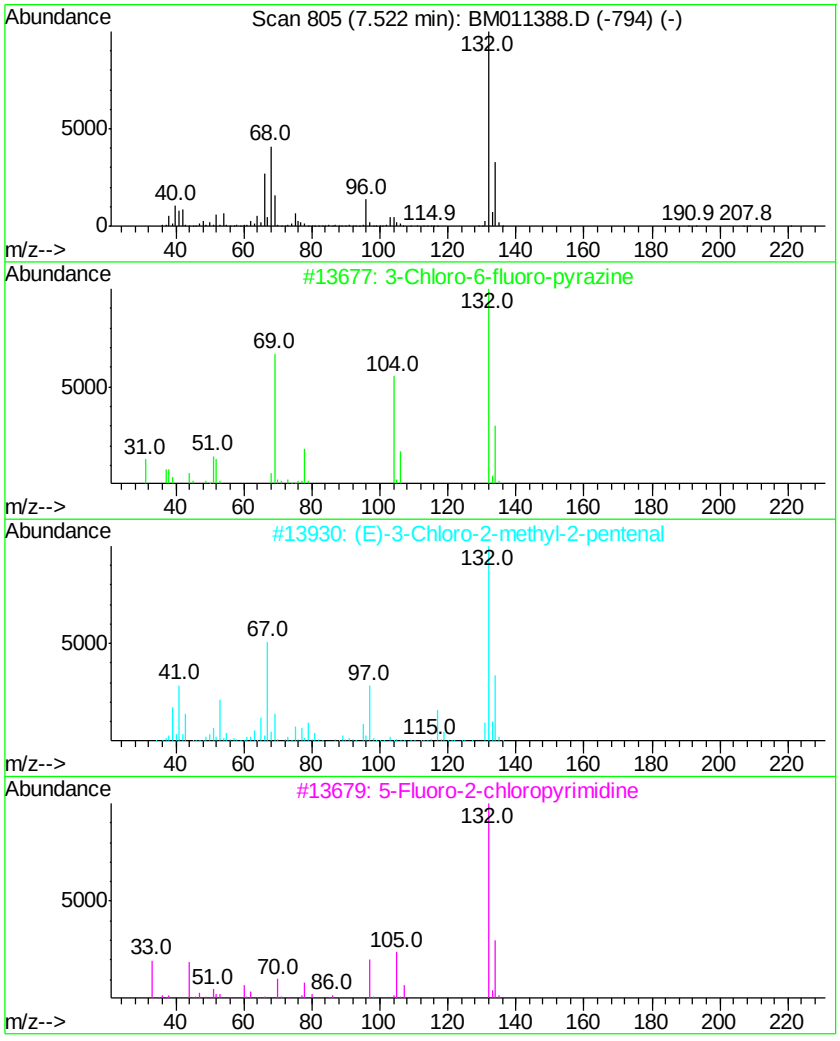
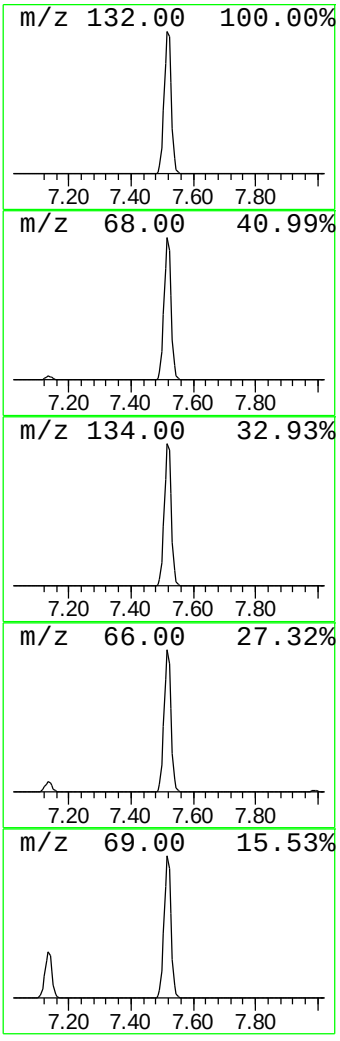
Peak Number 4 unknown7.52 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.52	92.49 ng	13803600	1,4-Dichlorobenzene-d4	7.99

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	17
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	5-Aminoindole	132	C8H8N2	005192-03-0	10





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Instrument : BNA_M
ClientSampleId : 3828-SPP4-DUP

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM083117.M
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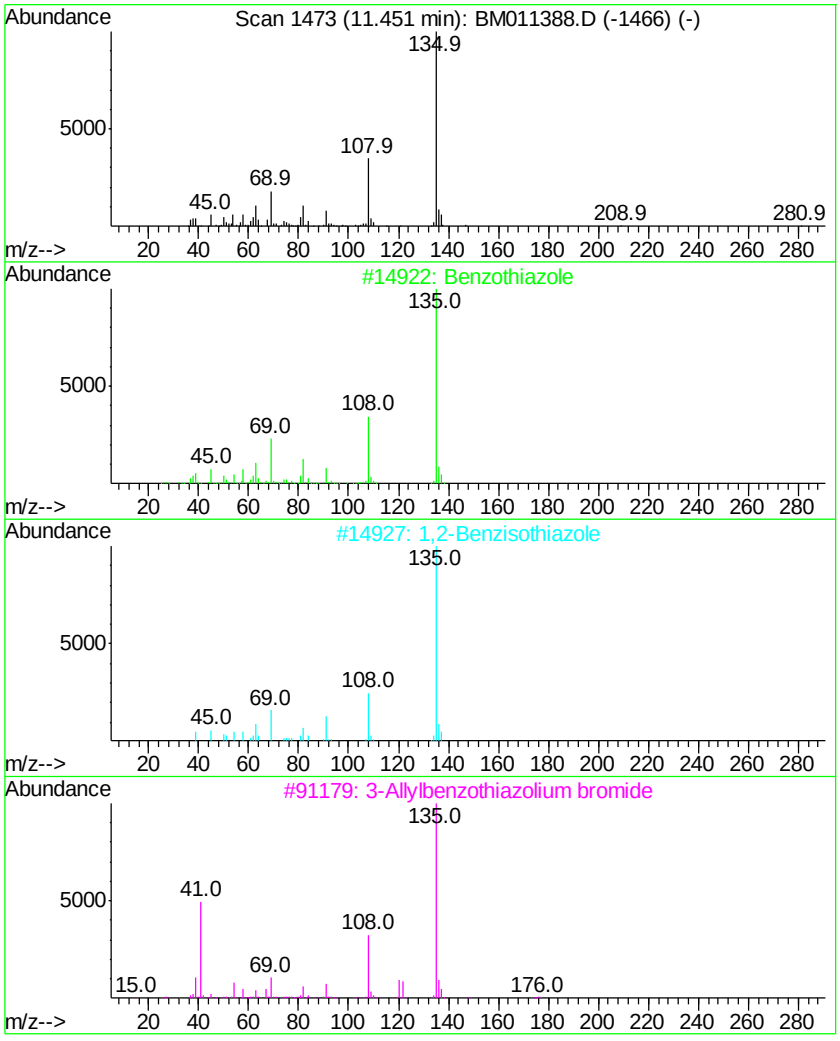
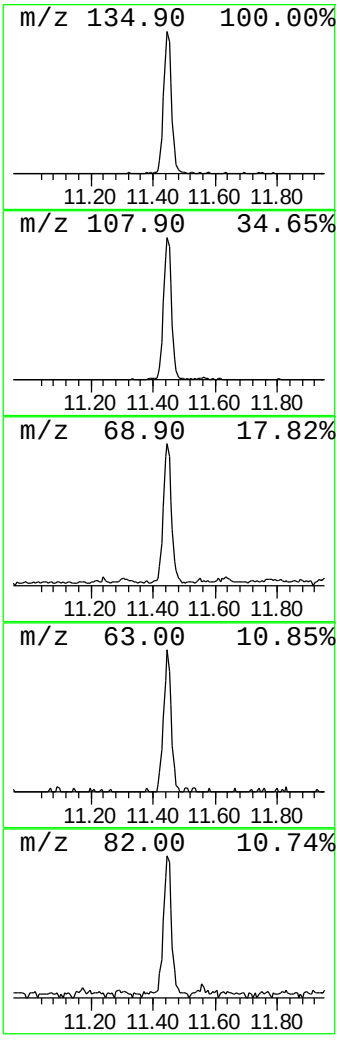
Peak Number 6 Benzothiazole Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.45	2.82 ng	627298	Naphthalene-d8	10.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzothiazole	135	C7H5NS	000095-16-9	97
2	1,2-Benzisothiazole	135	C7H5NS	000272-16-2	91
3	3-Allylbenzothiazolium bromide	255	C10H10BrNS	016407-55-9	64
4	1H-Pyrazolo[3,4-d]pyrimidin-4-amine	135	C5H5N5	002380-63-4	53
5	4-Methoxybenzenamine, N-(4-benzy...	360	C22H20N2O3	302909-73-5	50





Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Cyclohexane	3.06	14.5	ng	2160740	1	7.99	2984830	20.0
Butane, 2-methoxy...	3.13	4.4	ng	659663	1	7.99	2984830	20.0
2-Pentanone, 4-hy...	5.08	3.1	ng	456544	1	7.99	2984830	20.0
unknown7.52	7.52	92.5	ng	13803600	1	7.99	2984830	20.0
Benzothiazole	11.45	2.8	ng	627298	2	10.80	4442590	20.0