LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF111414\
Data File : BF075589.D
Acq On : 16 Nov 2014 19:44
Operator : TP / JJ
Sample : PB80336BL
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB80336BL

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-BF111214.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	1.624	45	47	50	rVB	207202	234055	19.16%	2.223%
2	1.761	56	59	63	rVB2	25860	57532	4.71%	0.546%
3	1.830	63	65	75	rVV	192904	381715	31.25%	3.625%
4	1.967	75	77	98	rVB	656347	1121142	91.80%	10.646%
5	4.573	303	305	309	rBV	89112	118269	9.68%	1.123%
6	5.350	370	373	376	rBV	938607	1221303	100.00%	11.597%
7	5.853	414	417	419	rBV	477180	484692	39.69%	4.603%
8	6.344	458	460	463	rVB	45072	41941	3.43%	0.398%
9	7.099	524	526	529	rBV	445841	473368	38.76%	4.495%
10	7.259	538	540	543	rBV	416853	492627	40.34%	4.678%
11	7.556	563	566	568	rBV	182724	181310	14.85%	1.722%
12	7.739	580	582	584	rVB	694073	620316	50.79%	5.890%
13	8.242	624	626	629	rBV	565762	488160	39.97%	4.635%
14	9.133	702	704	706	rBV	296730	254000	20.80%	2.412%
15	10.482	819	822	824	rBV	952133	950188	77.80%	9.023%
16	11.316	892	895	897	rBV	285790	271099	22.20%	2.574%
17	12.299	978	981	984	rBV	301841	357061	29.24%	3.391%
18	13.168	1054	1057	1059	rBV	269907	295002	24.15%	2.801%
19	15.157	1228	1231	1234	rBV	1147969	1158634	94.87%	11.002%
20	16.460	1343	1345	1348	rBV	293883	350803	28.72%	3.331%
21	17.397	1418	1427	1434	rBV	151456	515914	42.24%	4.899%
22	17.911	1470	1472	1477	rVB6	4286	12684	1.04%	0.120%
23	18.231	1497	1500	1506	rBV	326162	449200	36.78%	4.265%

Sum of corrected areas: 10531015

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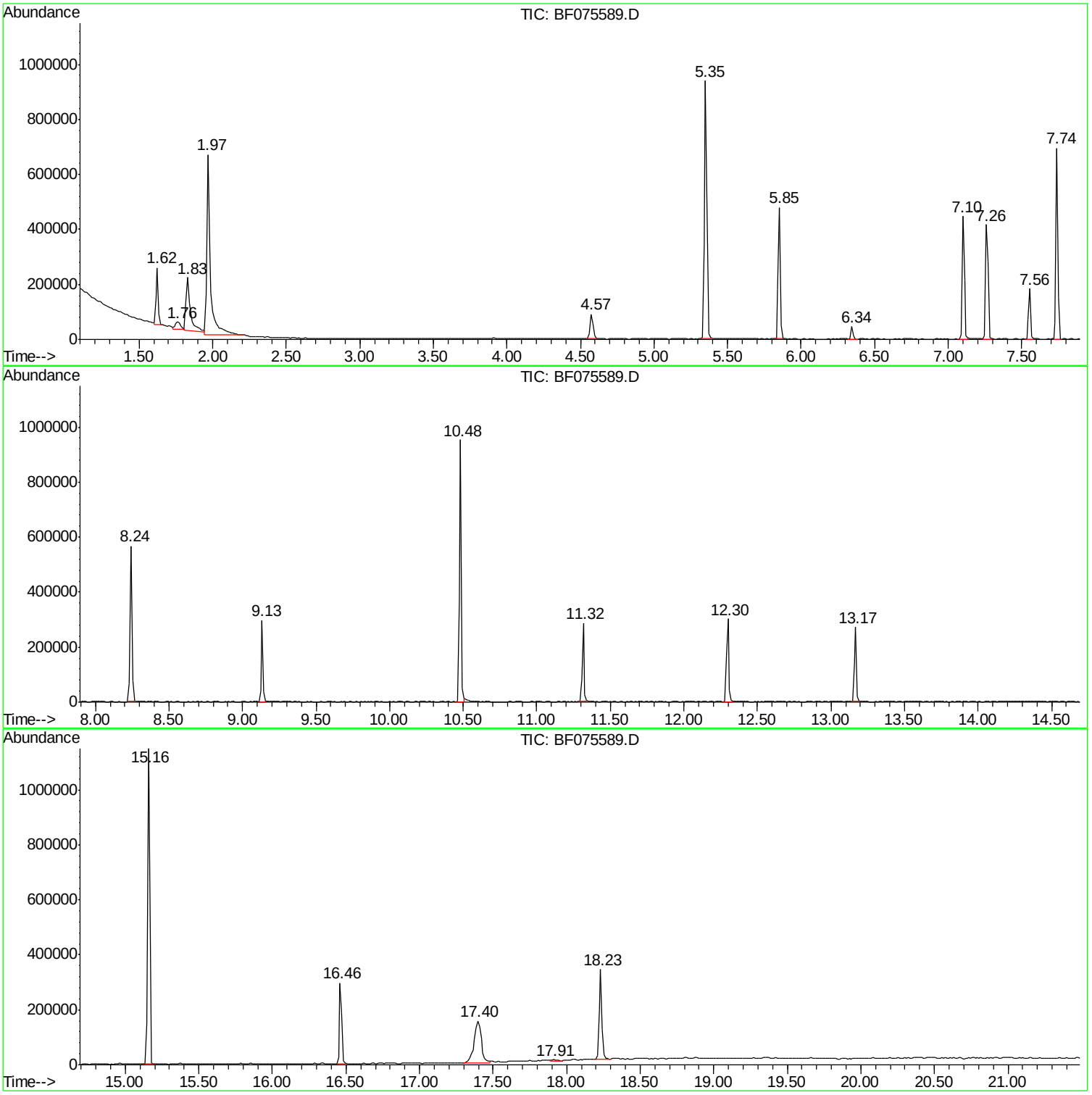
BNA_F
ClientSampleId :
PB80336BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF111214.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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Data File : BF075589.D
Acq On : 16 Nov 2014 19:44
Operator : TP / JJ
Sample : PB80336BL
Misc :
ALS Vial : 16 Sample Multiplier: 1

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

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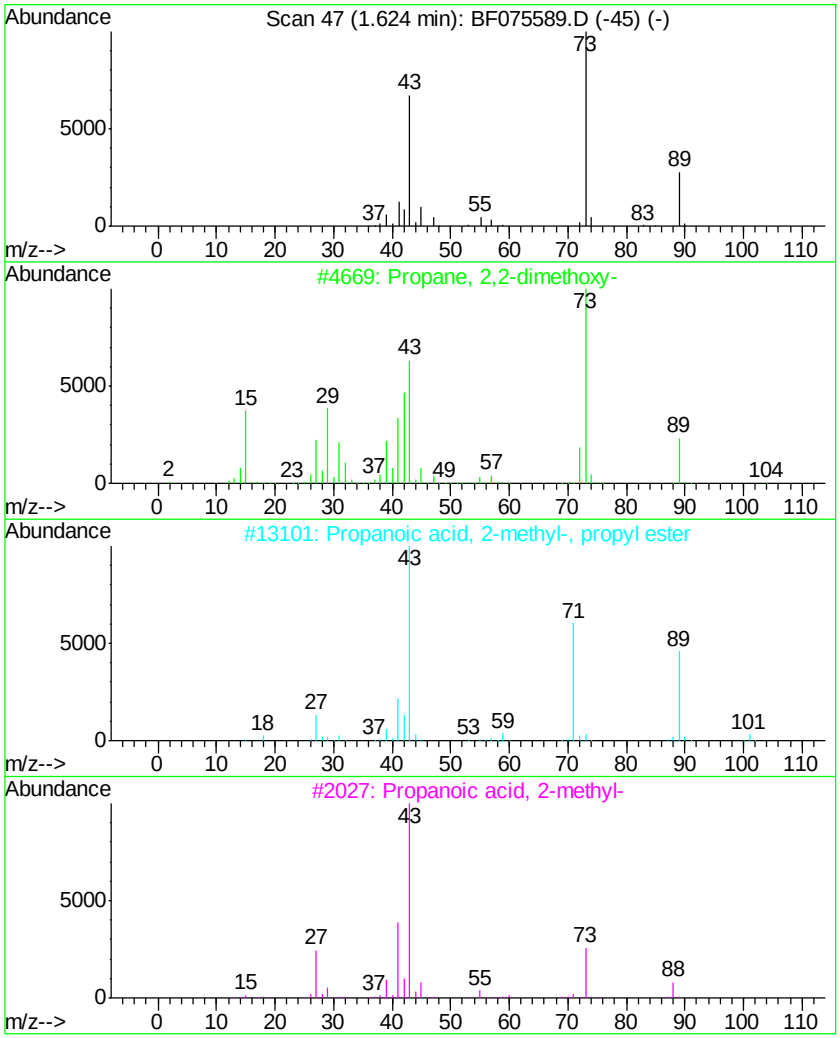
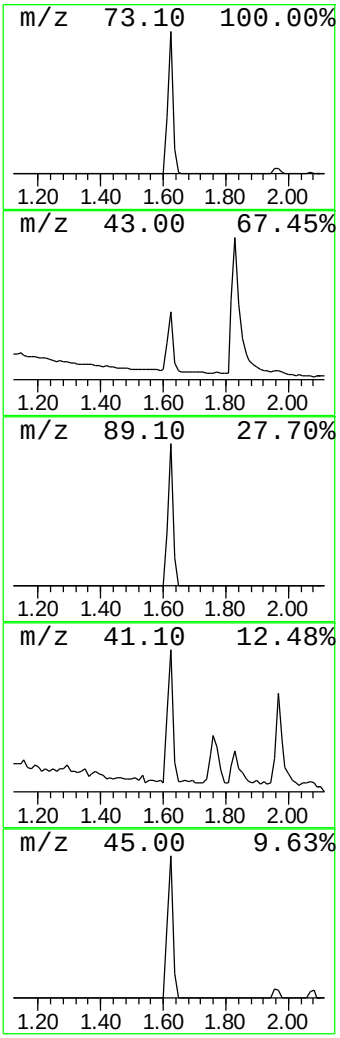
Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.62	25.82 ng	234055	1,4-Dichlorobenzene-d4	7.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	50
2	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	23
3	Propanoic acid, 2-methyl-	88	C4H8O2	000079-31-2	9
4	2-Butanone, 3-methoxy-3-methyl-	116	C6H12O2	036687-98-6	9
5	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9





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Sample : PB80336BL
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB80336BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF111214.M
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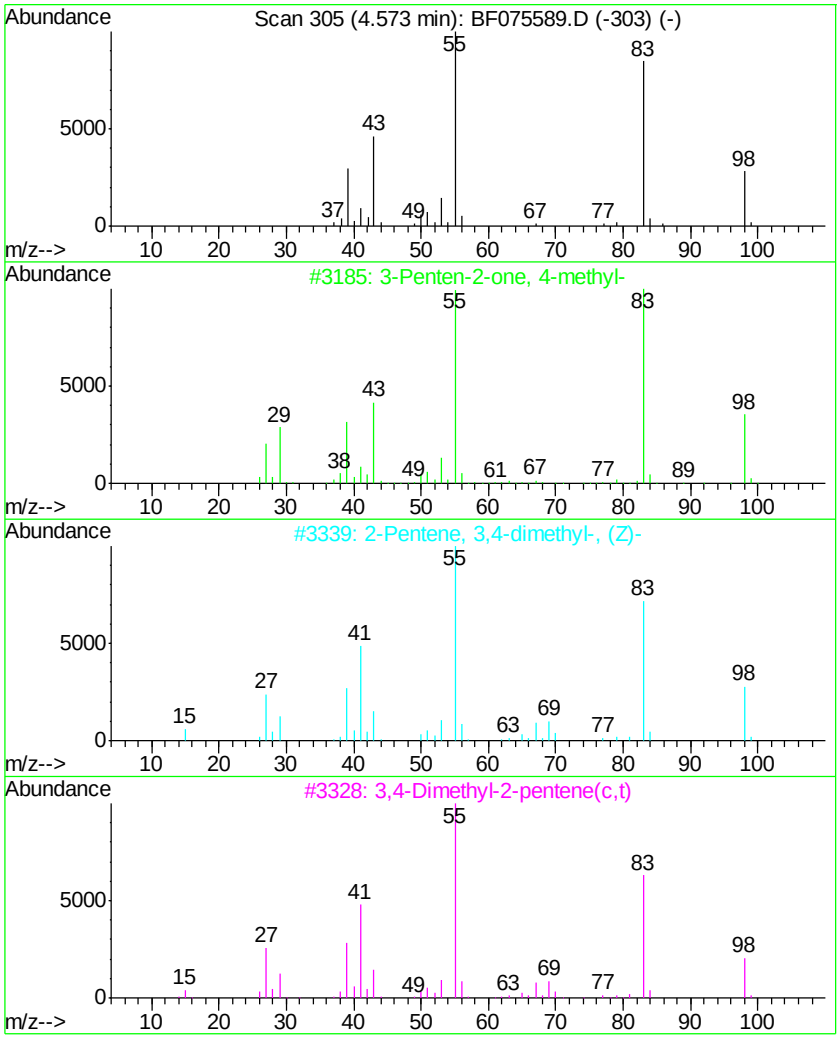
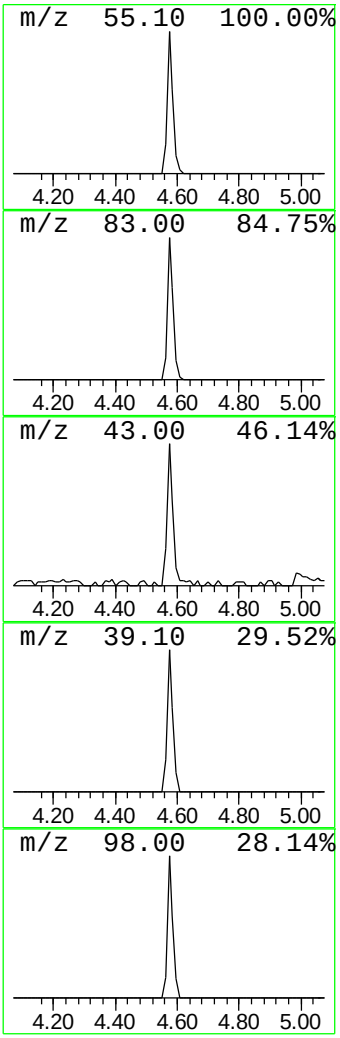
Peak Number 5 3-Penten-2-one, 4-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.57	13.05 ng	118269	1,4-Dichlorobenzene-d4	7.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
3	3,4-Dimethyl-2-pentene(c,t)	98	C7H14	1000118-16-5	86
4	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
5	3-Hexen-2-one	98	C6H10O	000763-93-9	80





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF111414\
Data File : BF075589.D
Acq On : 16 Nov 2014 19:44
Operator : TP / JJ
Sample : PB80336BL
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB80336BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF111214.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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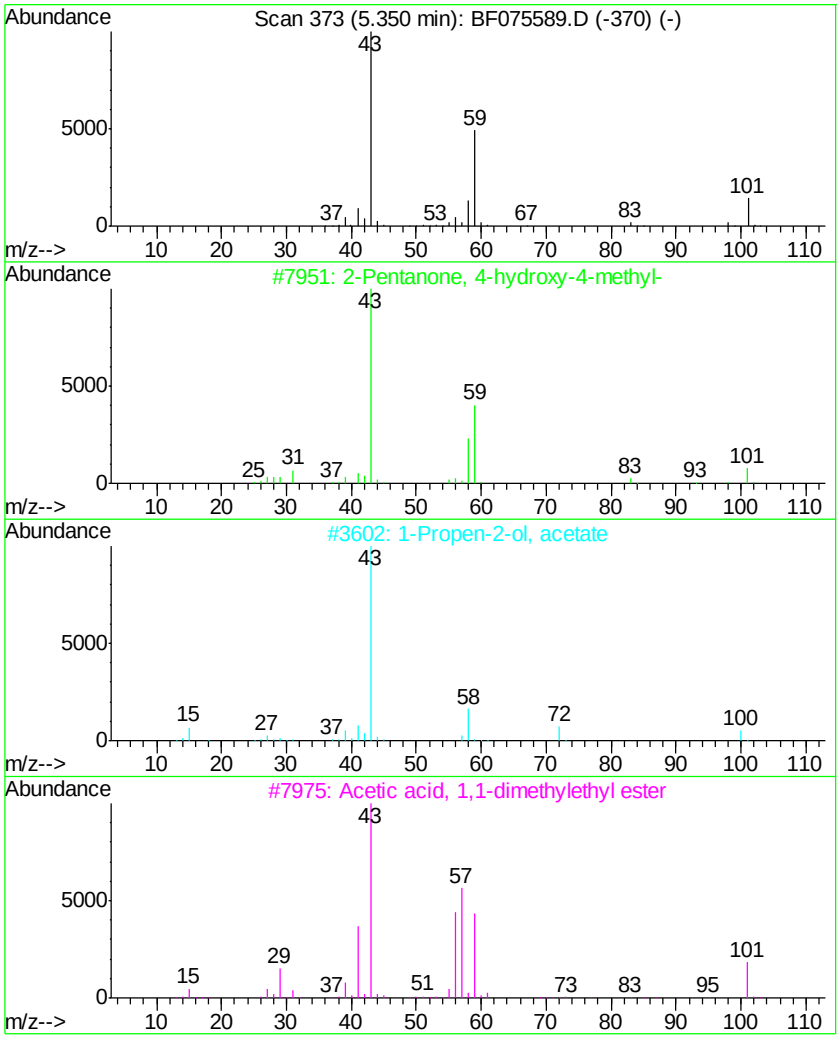
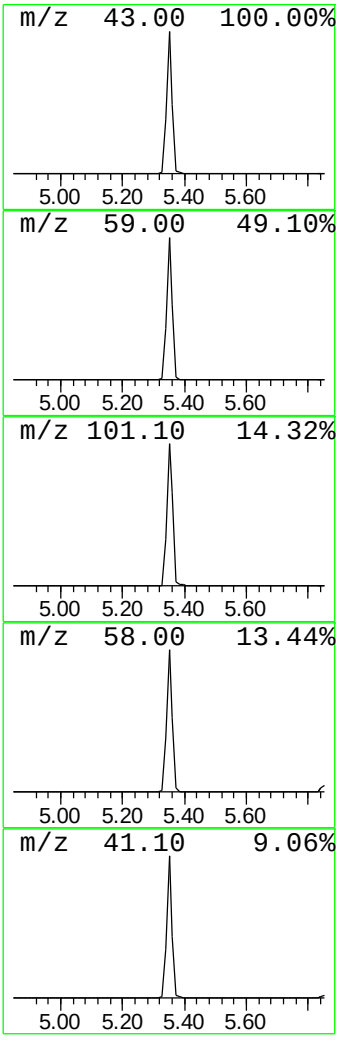
Peak Number 6 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.35	134.72 ng	1221300	1,4-Dichlorobenzene-d4	7.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9
4	Formamide, N,N-diethyl-	101	C5H11NO	000617-84-5	7
5	2-Propyn-1-ol, acetate	98	C5H6O2	000627-09-8	5





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ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB80336BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF111214.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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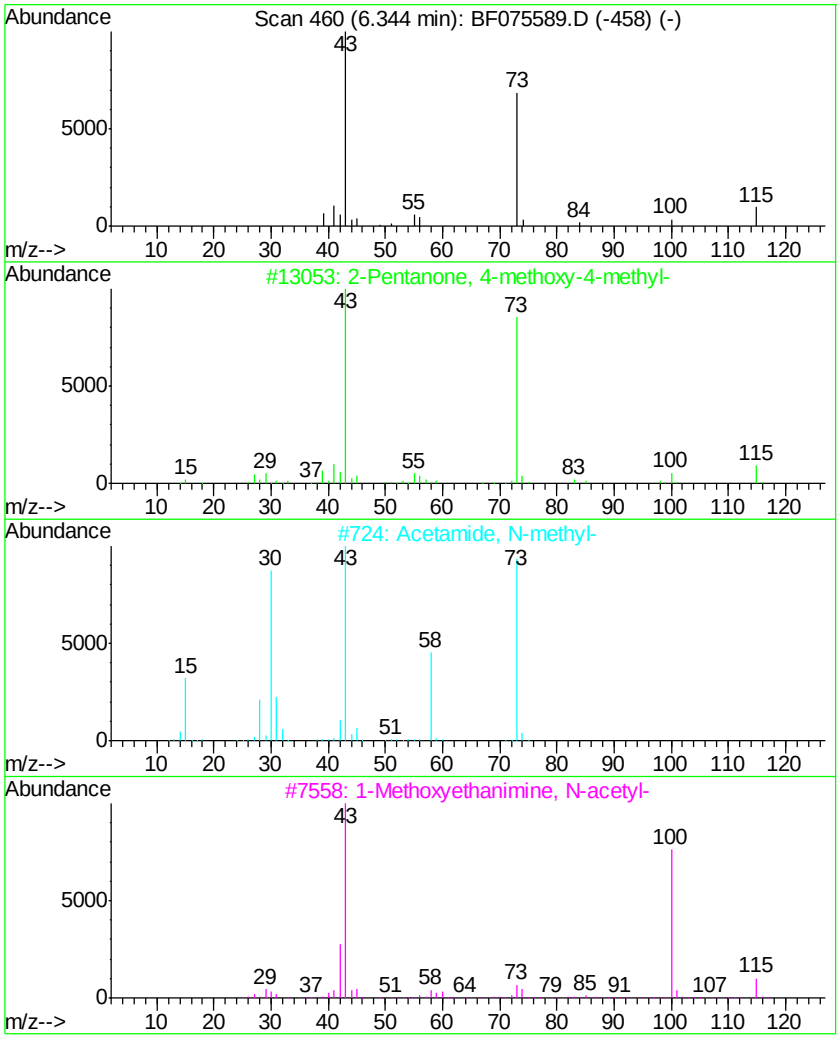
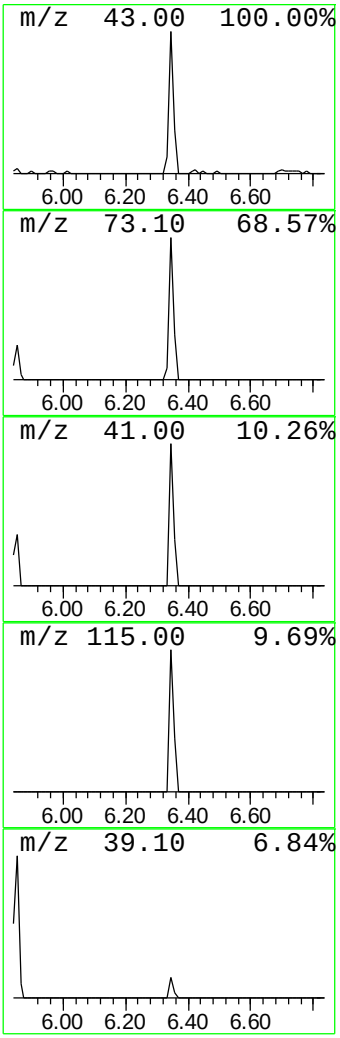
Peak Number 7 2-Pentanone, 4-methoxy-4-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.34	4.63 ng	41941	1,4-Dichlorobenzene-d4	7.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	59
2	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9
3	1-Methoxyethanimine, N-acetyl-	115	C5H9NO2	099028-43-0	9
4	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
5	5-Aminovaleric acid	117	C5H11NO2	000660-88-8	9





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ALS Vial : 16 Sample Multiplier: 1

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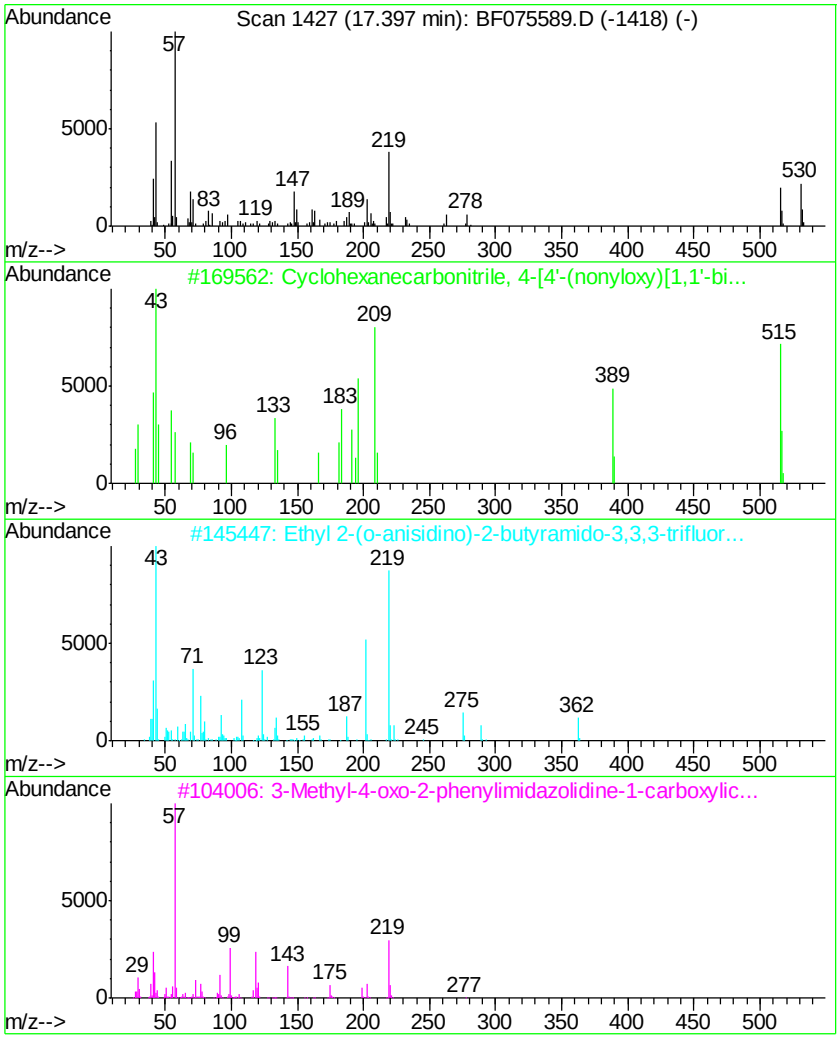
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

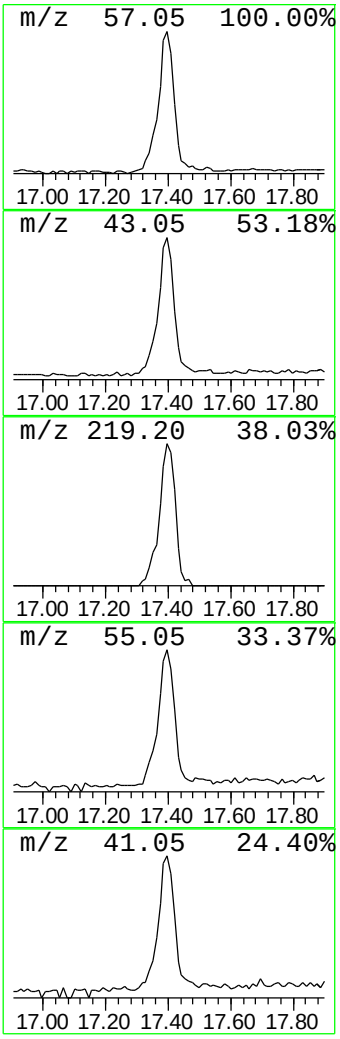
****

Peak Number 10 unknown17.40 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.40	22.97 ng	515914	Perylene-d12	18.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanecarbonitrile, 4-[4'-(...	515	C36H53NO	124729-19-7	11
2	Ethyl 2-(o-anisidino)-2-butyrami...	362	C16H21F3N2O4	339352-54-4	9
3	3-Methyl-4-oxo-2-phenylimidazoli...	276	C15H20N2O3	1000191-10-7	9
4	5-[1-(4-Isobutyl-phenyl)-ethyl]-...	261	C14H19N3S	1000296-89-6	9
5	2,2-Dimethyl-N-(2,2,2-trichloro-...	336	C14H19Cl3N2O	300382-25-6	4





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
Propane, 2,2-dime...	1.62	25.8	ng	234055	1	7.56	181310	20.0
3-Penten-2-one, 4...	4.57	13.1	ng	118269	1	7.56	181310	20.0
2-Pentanone, 4-hy...	5.35	134.7	ng	1221300	1	7.56	181310	20.0
2-Pentanone, 4-me...	6.34	4.6	ng	41941	1	7.56	181310	20.0
unknown17.40	17.40	23.0	ng	515914	6	18.23	449200	20.0