LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF051515\
Data File : BF079273.D
Acq On : 15 May 2015 16:49
Operator : TP/IZ
Sample : PB83262BL
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB83262BL

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-BF043015.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	1.347	12	14	17	rVB	305729	306317	13.91%	1.778%
2	1.667	41	42	48	rBV	162704	278101	12.63%	1.614%
3	1.793	51	53	77	rVB	492370	958997	43.55%	5.565%
4	4.136	256	258	265	rVB	52637	78037	3.54%	0.453%
5	4.947	327	329	337	rVB	319087	383181	17.40%	2.224%
6	5.473	372	375	377	rBV	1204537	1446109	65.68%	8.392%
7	6.742	484	486	489	rBV	1291789	1380067	62.68%	8.009%
8	6.890	496	499	501	rBV	1535392	1555167	70.63%	9.025%
9	7.176	521	524	527	rVB	426883	381035	17.31%	2.211%
10	7.359	538	540	543	rBV	1142743	1153544	52.39%	6.695%
11	7.873	582	585	587	rBV	869890	923160	41.93%	5.358%
12	8.753	660	662	664	rBV	581138	526626	23.92%	3.056%
13	10.102	777	780	782	rBV	1998045	1852398	84.13%	10.750%
14	10.925	850	852	855	rVB	642425	594656	27.01%	3.451%
15	11.908	935	938	940	rBV	991853	1229120	55.82%	7.133%
16	12.765	1010	1013	1015	rBV	660472	614080	27.89%	3.564%
17	14.765	1185	1188	1190	rBV	1984656	2201856	100.00%	12.778%
18	16.068	1300	1302	1305	rBV	547661	616883	28.02%	3.580%
19	17.783	1448	1452	1455	rBV3	21835	72012	3.27%	0.418%
20	17.840	1455	1457	1460	rVV	35782	83140	3.78%	0.482%
21	17.897	1460	1462	1465	rVB	452545	596665	27.10%	3.463%

Sum of corrected areas: 17231151

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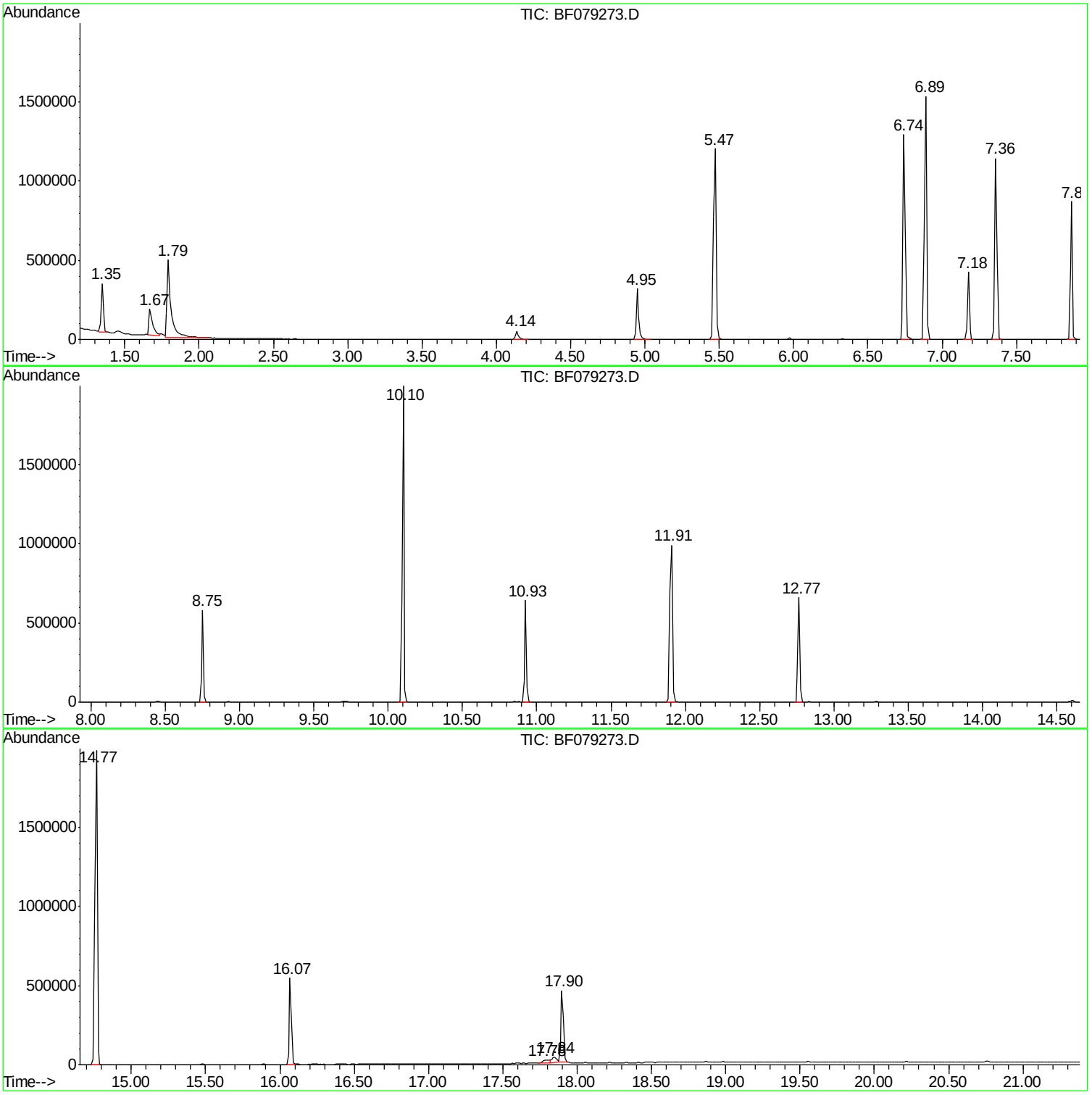
BNA_F
ClientSampleId :
PB83262BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF043015.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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Operator : TP/IZ
Sample : PB83262BL
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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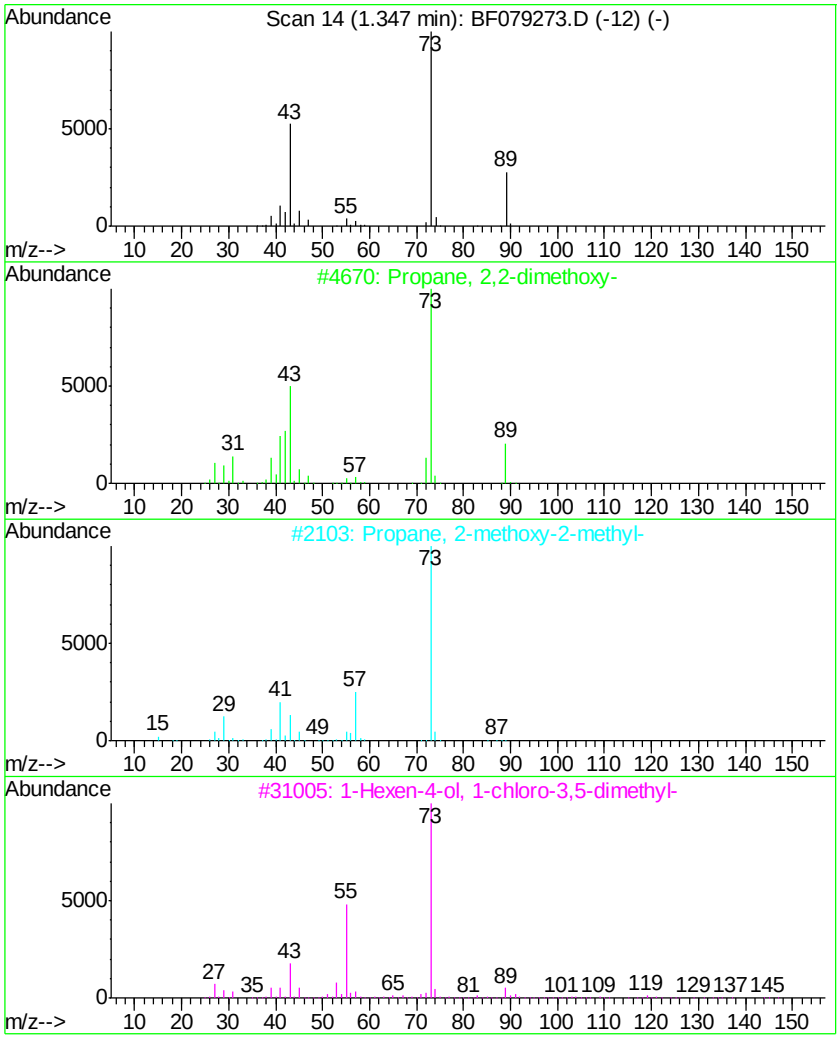
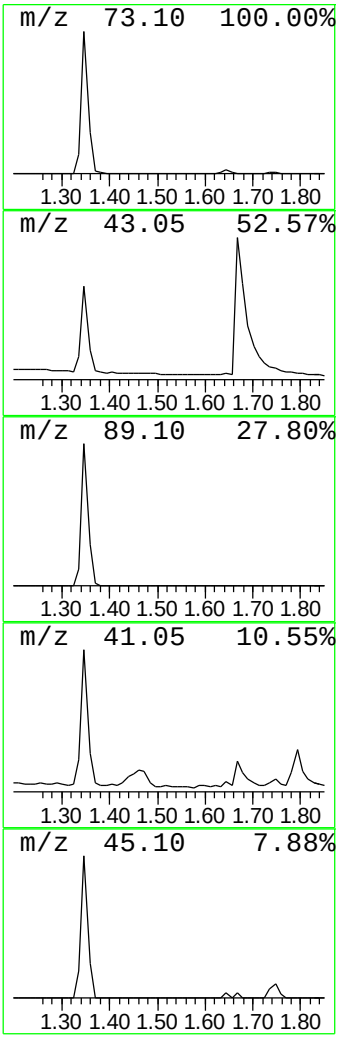
Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.35	16.08 ng	306317	1,4-Dichlorobenzene-d4	7.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	72
2	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
3	1-Hexen-4-ol, 1-chloro-3,5-dimet...	162	C8H15ClO	100244-09-5	9
4	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	9
5	1,3-Diaminoguanidine	89	CH7N5	004364-78-7	7





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Operator : TP/IZ
Sample : PB83262BL
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB83262BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF043015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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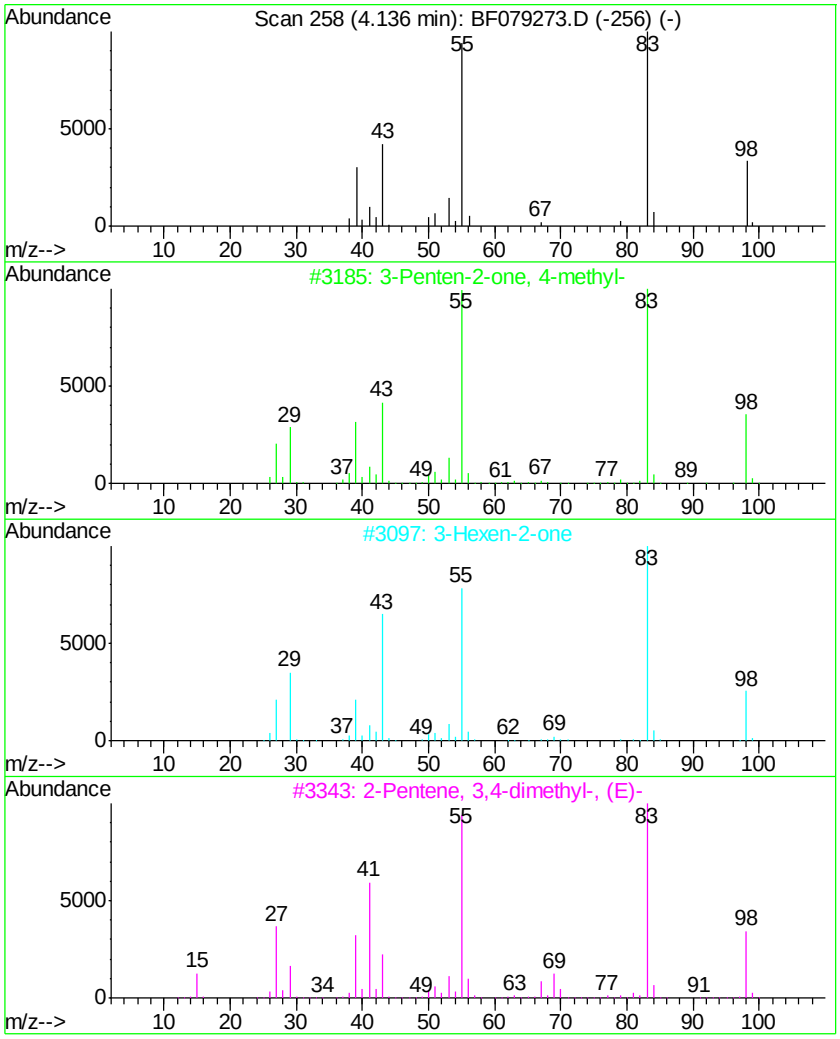
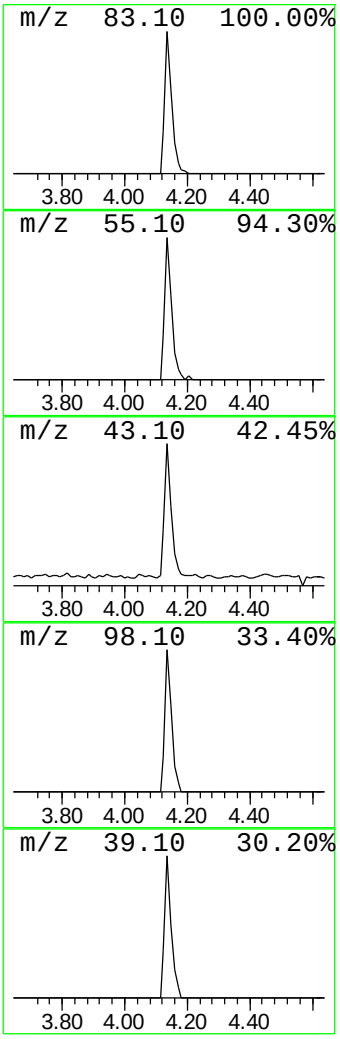
Peak Number 4 3-Penten-2-one, 4-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.14	4.10 ng	78037	1,4-Dichlorobenzene-d4	7.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2	3-Hexen-2-one	98	C6H10O	000763-93-9	87
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
4	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80
5	2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	80





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF051515\
Data File : BF079273.D
Acq On : 15 May 2015 16:49
Operator : TP/IZ
Sample : PB83262BL
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB83262BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF043015.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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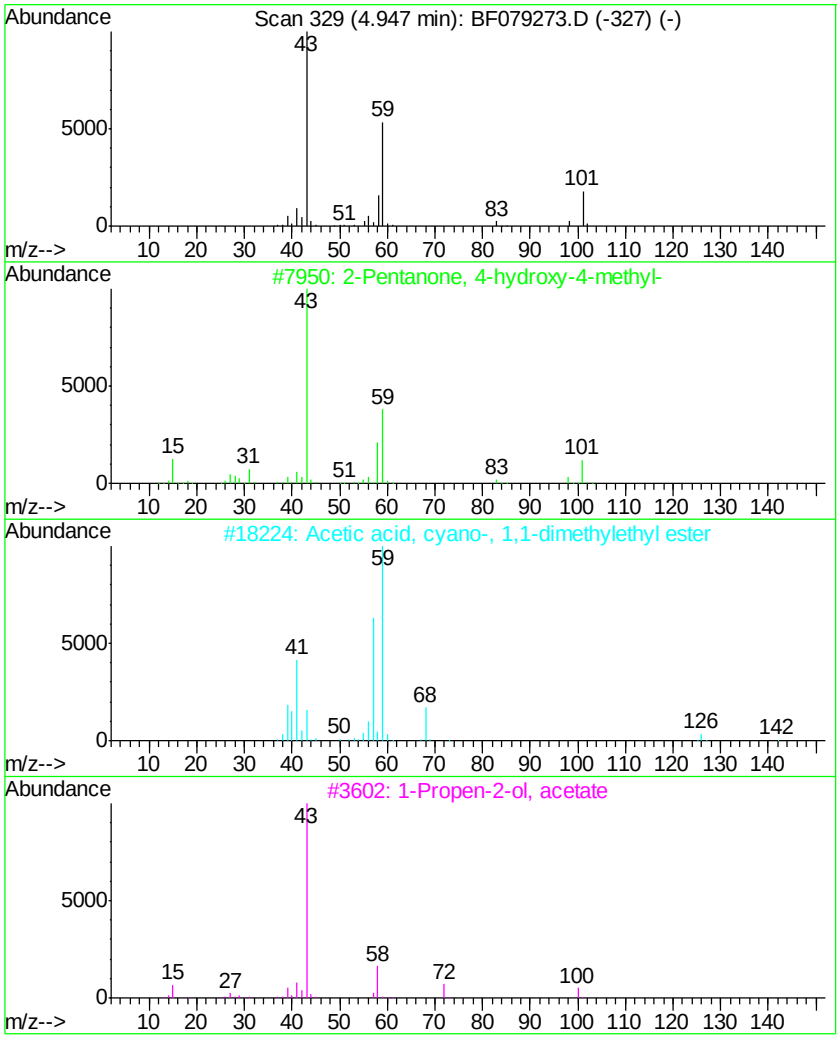
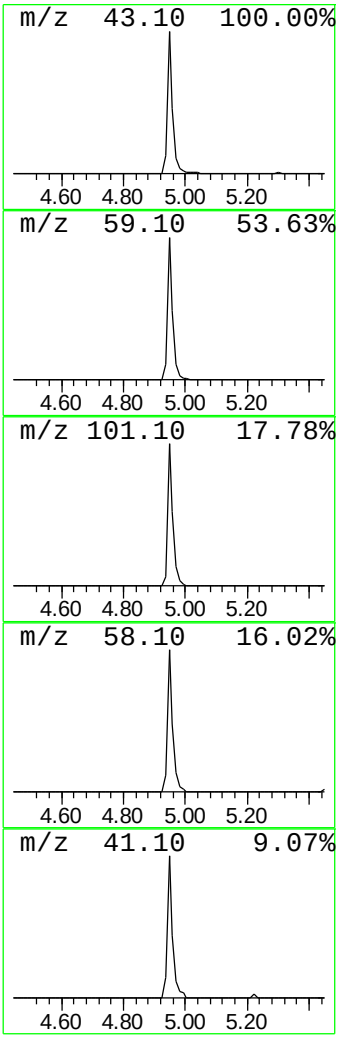
Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.95	20.11 ng	383181	1,4-Dichlorobenzene-d4	7.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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ClientSampleId : PB83262BL

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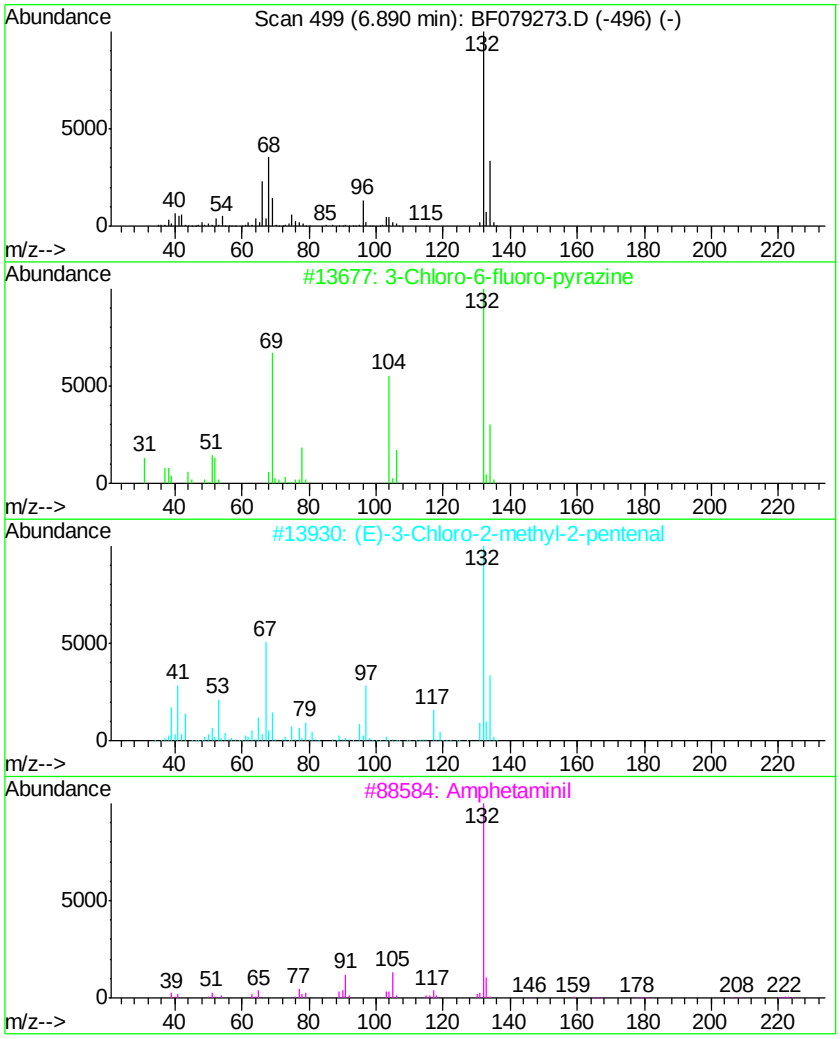
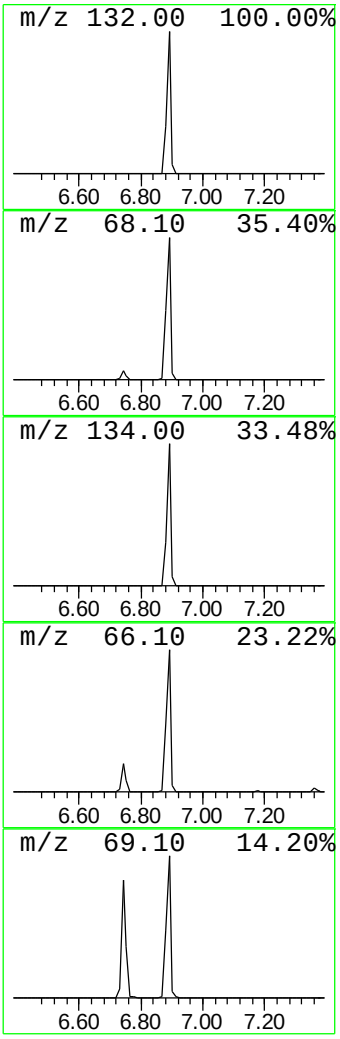
Peak Number 6 unknown6.89 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.89	81.63 ng	1555170	1,4-Dichlorobenzene-d4	7.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	Amphetaminil	250	C17H18N2	017590-01-1	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5	5-Aminoindole	132	C8H8N2	005192-03-0	12





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Instrument : BNA_F
ClientSampleId : PB83262BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF043015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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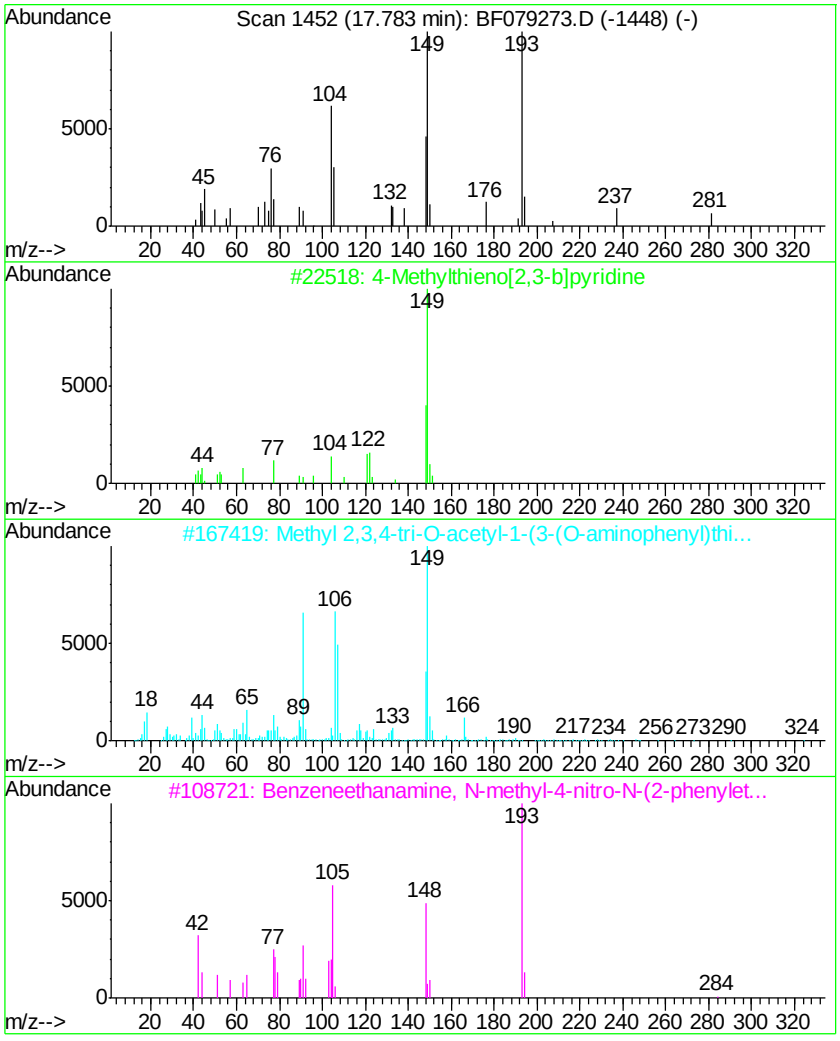
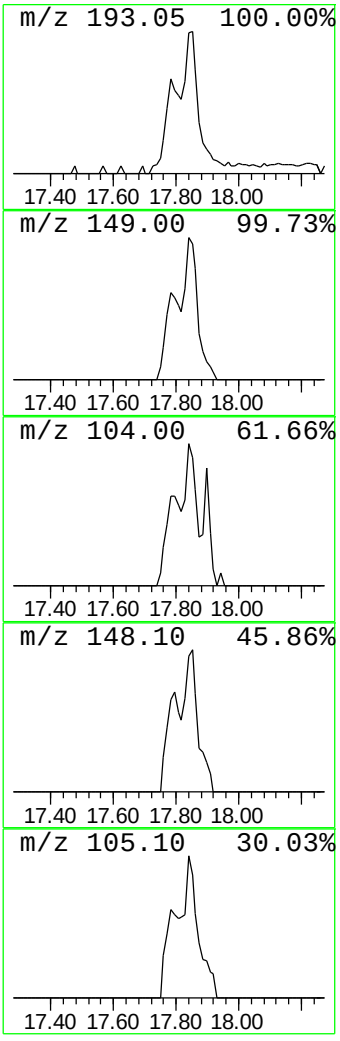
Peak Number 8 unknown17.78 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.78	2.41 ng	72012	Perylene-d12	17.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Methylthieno[2,3-b]pyridine	149	C8H7NS	013362-81-7	35
2	Methyl 2,3,4-tri-O-acetyl-1-(3-(...	483	C20H25N3O9S	1000242-58-9	25
3	Benzeneethanamine, N-methyl-4-ni...	284	C17H20N2O2	052118-15-7	23
4	Benzoic acid, 4-methyl-, tert-bu...	250	C14H22O2Si	345647-19-0	17
5	Benzene, 1-isothiocyanato-4-methyl-	149	C8H7NS	000622-59-3	17





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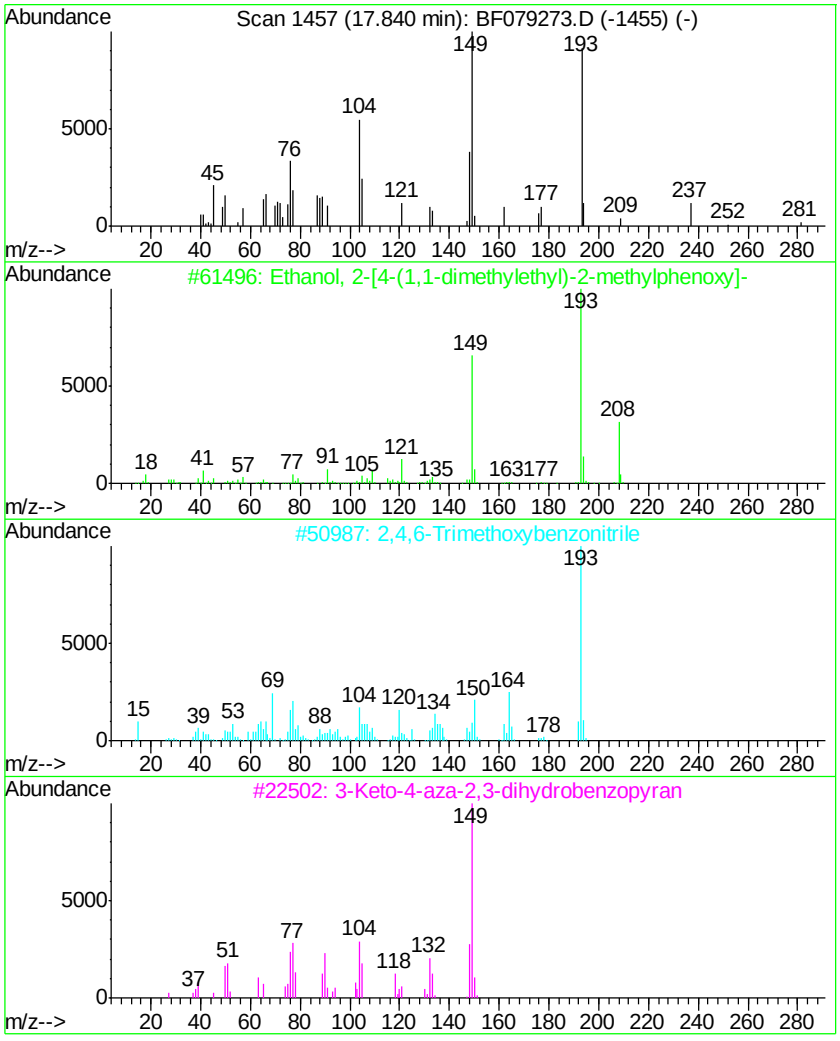
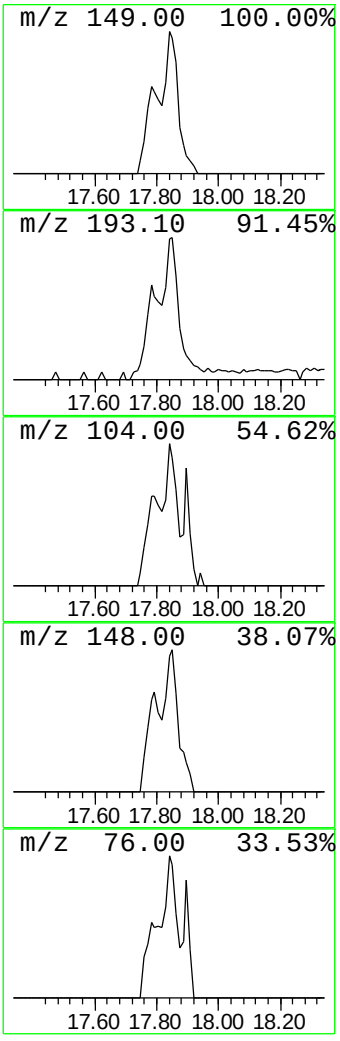
Peak Number 9 unknown17.84 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.84	2.79 ng	83140	Perylene-d12	17.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-[4-(1,1-dimethylethyl...	208	C13H20O2	054934-87-1	43
2	2,4,6-Trimethoxybenzonitrile	193	C10H11NO3	002571-54-2	32
3	3-Keto-4-aza-2,3-dihydrobenzopyran	149	C8H7NO2	1000289-12-0	32
4	Pentamethylnitrobenzene	193	C11H15NO2	013171-59-0	25
5	m-Tolualdehyde, thiosemicarbazone	193	C9H11N3S	005706-82-1	22





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...	1.35	16.1	ng	306317	1	7.18	381035	20.0
3-Penten-2-one, 4...	4.14	4.1	ng	78037	1	7.18	381035	20.0
2-Pentanone, 4-hy...	4.95	20.1	ng	383181	1	7.18	381035	20.0
unknown6.89	6.89	81.6	ng	1555170	1	7.18	381035	20.0
unknown17.78	17.78	2.4	ng	72012	6	17.90	596665	20.0
unknown17.84	17.84	2.8	ng	83140	6	17.90	596665	20.0