LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF042915\
Data File : BF078834.D
Acq On : 30 Apr 2015 3:15
Operator : TP/IZ
Sample : G2022-14
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-10-COMP

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-BF042815.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	1.278	6	8	27	rVB2	415803	2020218	29.85%	6.376%
2	1.530	27	30	32	rVB	4140938	5059968	74.76%	15.970%
3	1.667	40	42	51	rVB	264284	532558	7.87%	1.681%
4	1.781	51	52	57	rVV	398145	660418	9.76%	2.084%
5	1.850	57	58	62	rVV	129528	213965	3.16%	0.675%
6	1.918	62	64	103	rVB	3576016	6768262	100.00%	21.362%
7	5.187	348	350	359	rVB	135036	155181	2.29%	0.490%
8	5.679	390	393	395	rBV	841297	1097392	16.21%	3.464%
9	6.925	499	502	504	rBV	1390847	1295803	19.15%	4.090%
10	7.085	514	516	519	rBV	1083493	1209851	17.88%	3.818%
11	7.382	540	542	544	rBV	475141	415556	6.14%	1.312%
12	7.565	556	558	561	rVB	867548	903236	13.35%	2.851%
13	8.068	600	602	605	rBV	819340	717210	10.60%	2.264%
14	8.959	678	680	682	rBV	689924	594357	8.78%	1.876%
15	10.308	795	798	800	rBV	1521409	1486333	21.96%	4.691%
16	11.142	868	871	873	rBV	496796	651431	9.62%	2.056%
17	12.114	954	956	959	rBV	984964	976474	14.43%	3.082%
18	12.982	1030	1032	1037	rBV2	762241	845460	12.49%	2.668%
19	14.491	1162	1164	1166	rBV	224132	229260	3.39%	0.724%
20	14.777	1186	1189	1191	rBV	216846	247436	3.66%	0.781%
21	14.845	1193	1195	1197	rBV	394489	437158	6.46%	1.380%
22	14.982	1204	1207	1210	rBV	1994717	1903522	28.12%	6.008%
23	16.148	1307	1309	1316	rBV2	140497	246267	3.64%	0.777%
24	16.274	1317	1320	1322	rBV2	845249	1083480	16.01%	3.420%
25	17.543	1428	1431	1437	rBV	118947	359508	5.31%	1.135%
26	17.851	1456	1458	1461	rVB	74647	101135	1.49%	0.319%
27	17.920	1461	1464	1467	rVV	110126	146529	2.16%	0.462%
28	17.988	1467	1470	1479	rVB	786232	1043981	15.42%	3.295%
29	19.497	1599	1602	1608	rVB2	54402	134831	1.99%	0.426%
30	19.943	1638	1641	1647	rVB	62861	147422	2.18%	0.465%

Sum of corrected areas: 31684202

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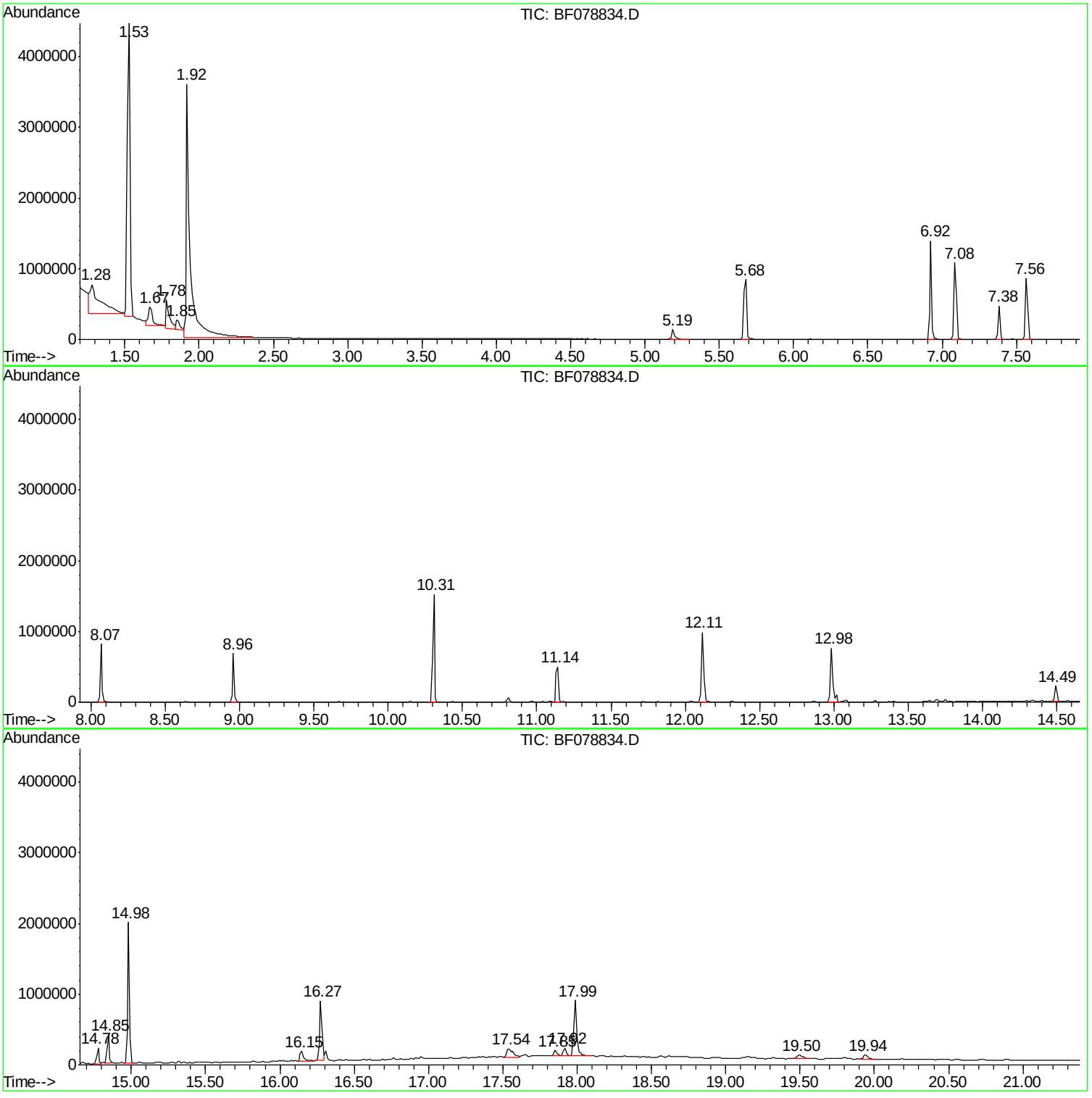
Instrument : BNA_F
ClientSampleId : SB-10-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042815.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

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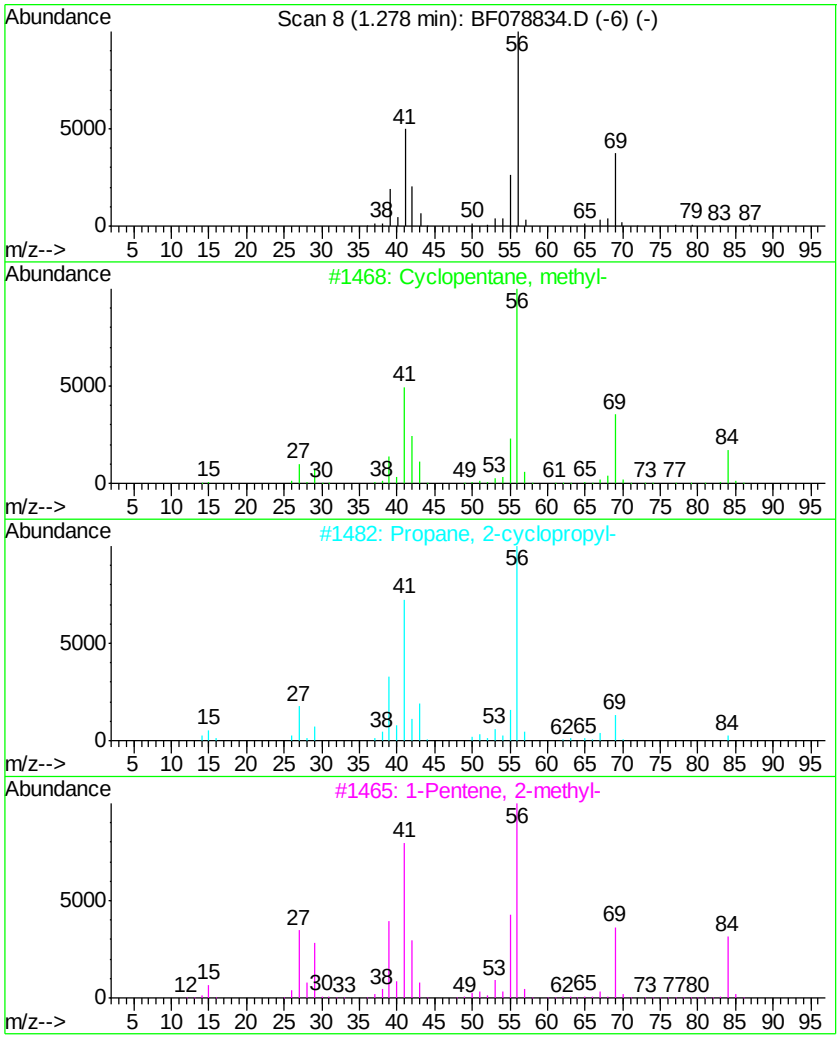
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

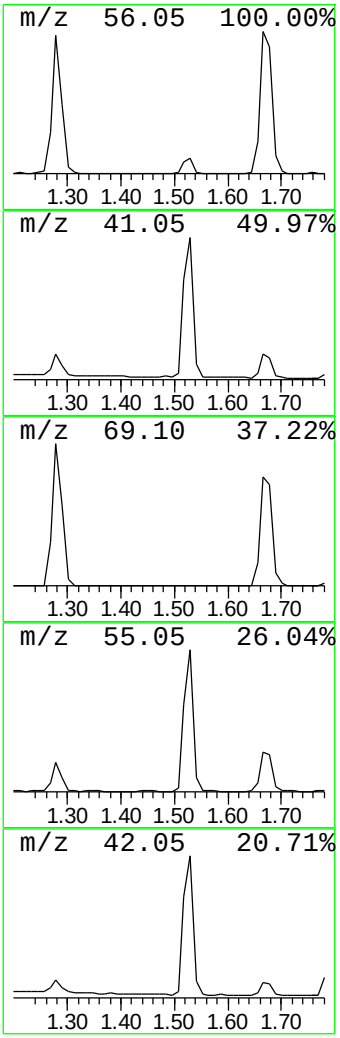
****

Peak Number 1 Cyclopentane, methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.28	97.23 ng	2020220	1,4-Dichlorobenzene-d4	7.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	83
2	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	56
3	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	50
4	Cyclobutane, ethyl-	84	C6H12	004806-61-5	43
5	Cyclopropane, propyl-	84	C6H12	002415-72-7	40





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF042915\
Data File : BF078834.D
Acq On : 30 Apr 2015 3:15
Operator : TP/IZ
Sample : G2022-14
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-10-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042815.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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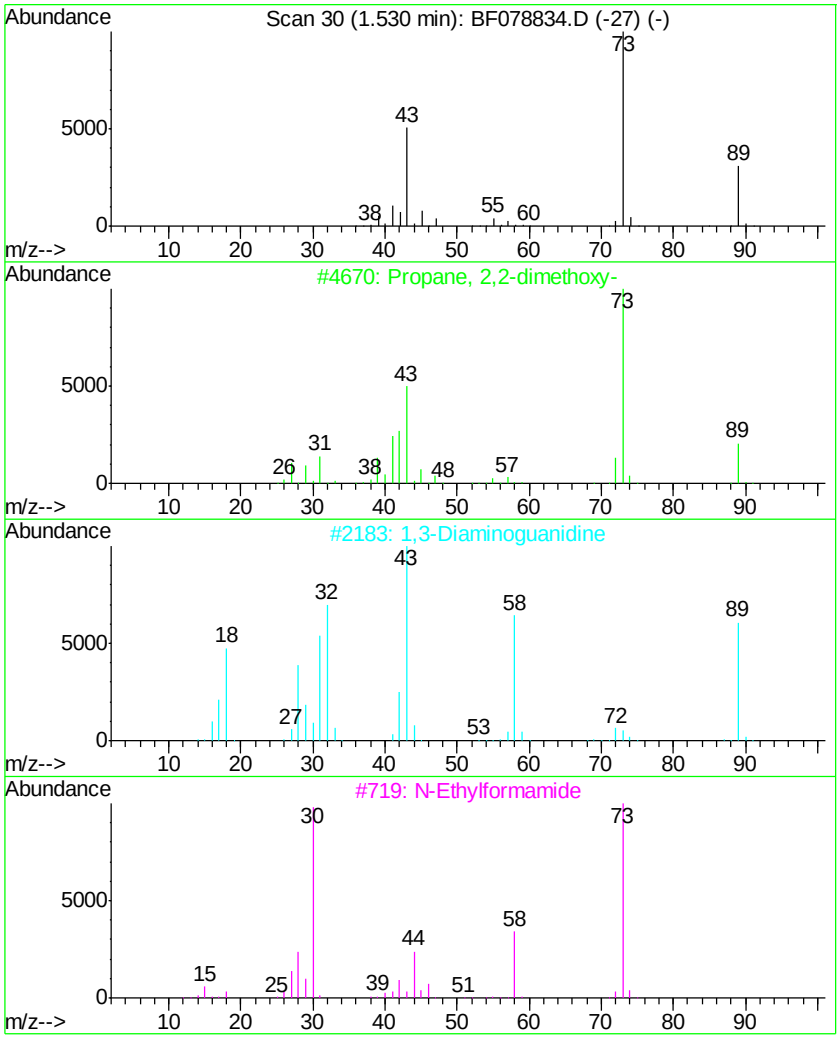
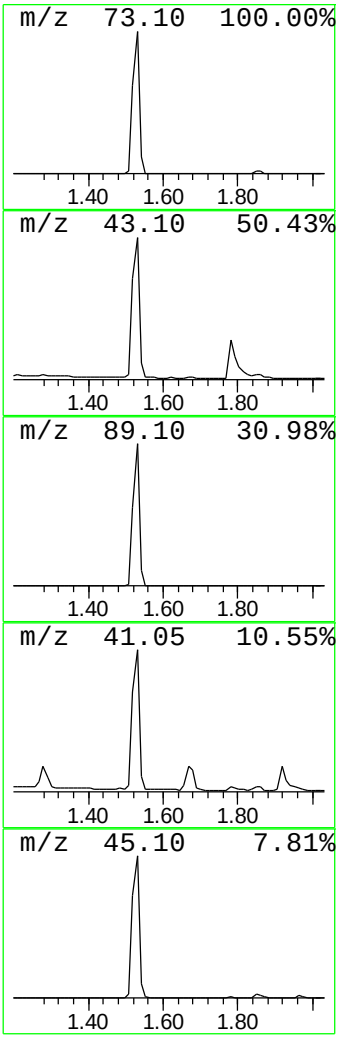
Peak Number 2 unknown1.53 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.53	243.53 ng	5059970	1,4-Dichlorobenzene-d4	7.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	38
2	1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9
3	N-Ethylformamide	73	C3H7NO	000627-45-2	9
4	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
5	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9





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Data File : BF078834.D
Acq On : 30 Apr 2015 3:15
Operator : TP/IZ
Sample : G2022-14
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-10-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042815.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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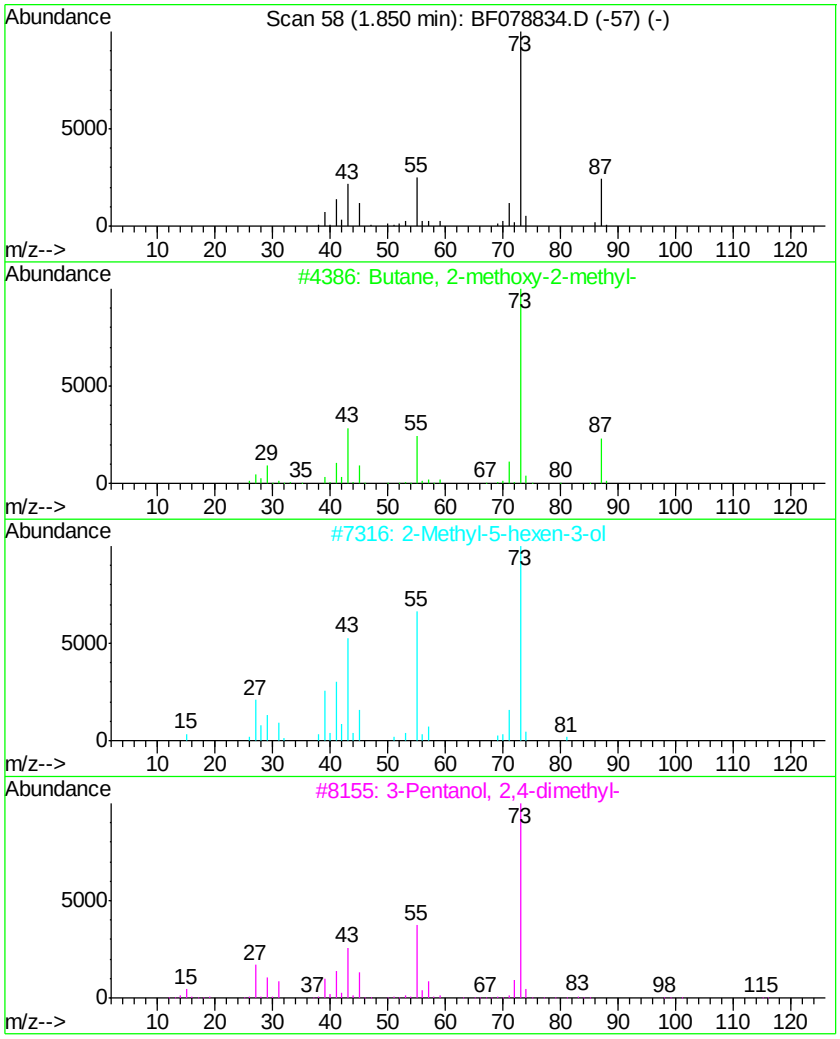
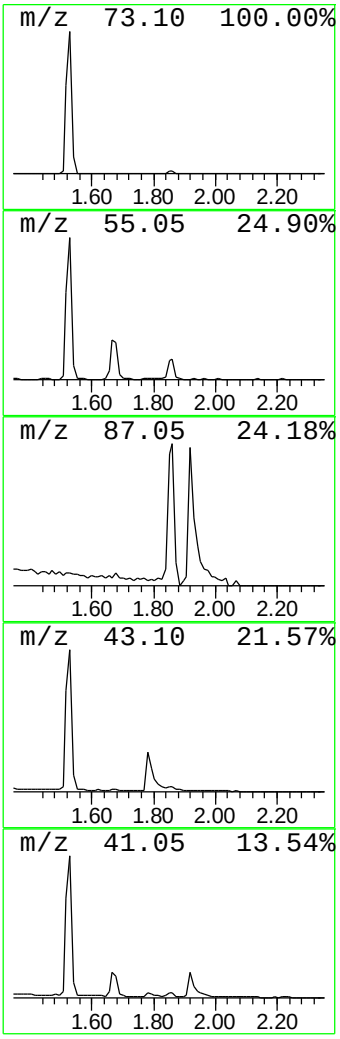
Peak Number 5 Butane, 2-methoxy-2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.85	10.30 ng	213965	1,4-Dichlorobenzene-d4	7.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	25
3	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	25
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5	1-Propene-1-thiol	74	C3H6S	000925-89-3	9





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Sample : G2022-14
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-10-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042815.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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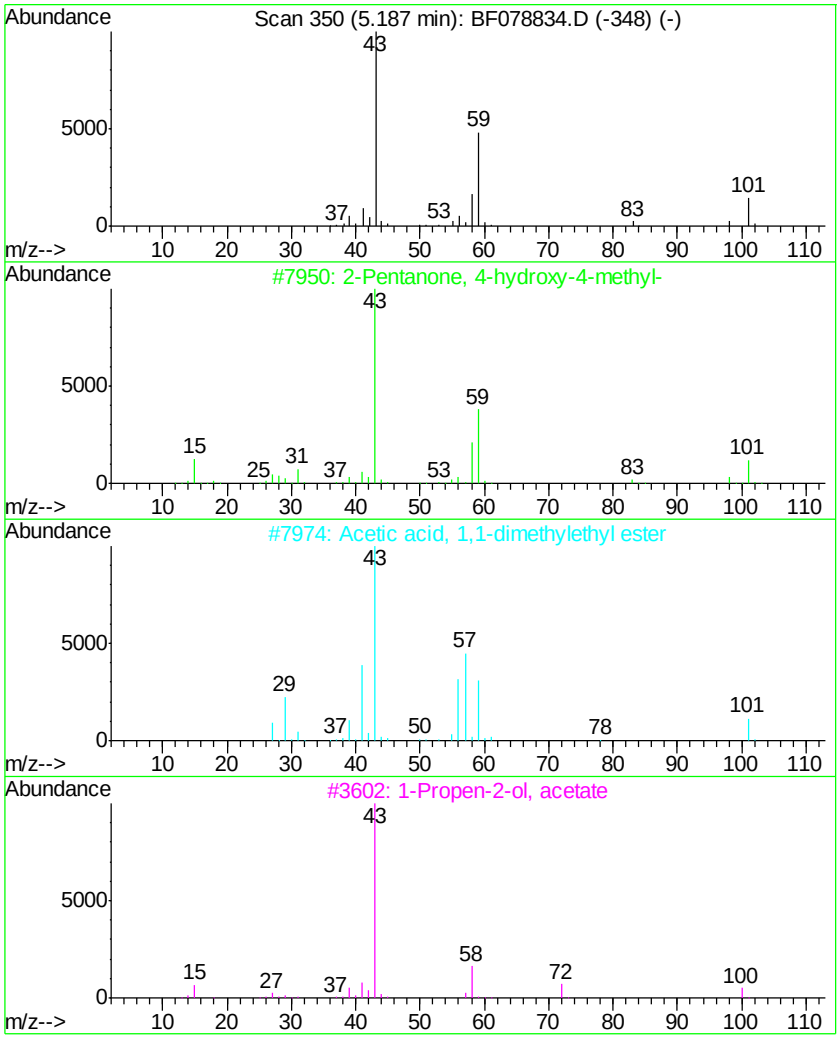
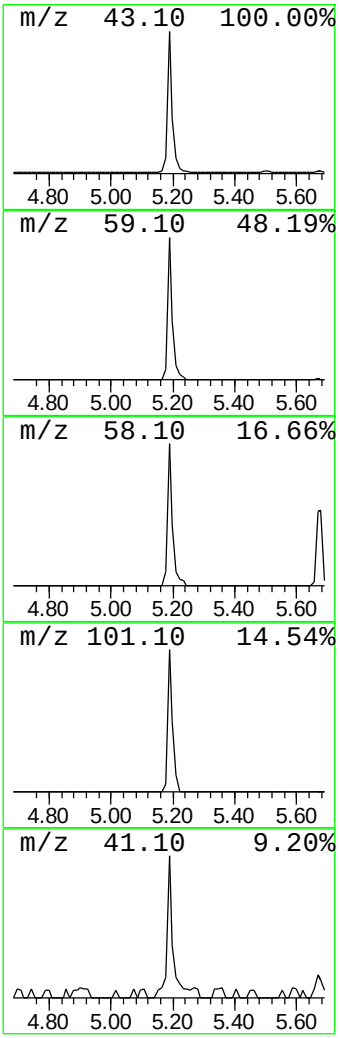
Peak Number 7 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	7.47 ng	155181	1,4-Dichlorobenzene-d4	7.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10
5	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9





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Data File : BF078834.D
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Operator : TP/IZ
Sample : G2022-14
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-10-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042815.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

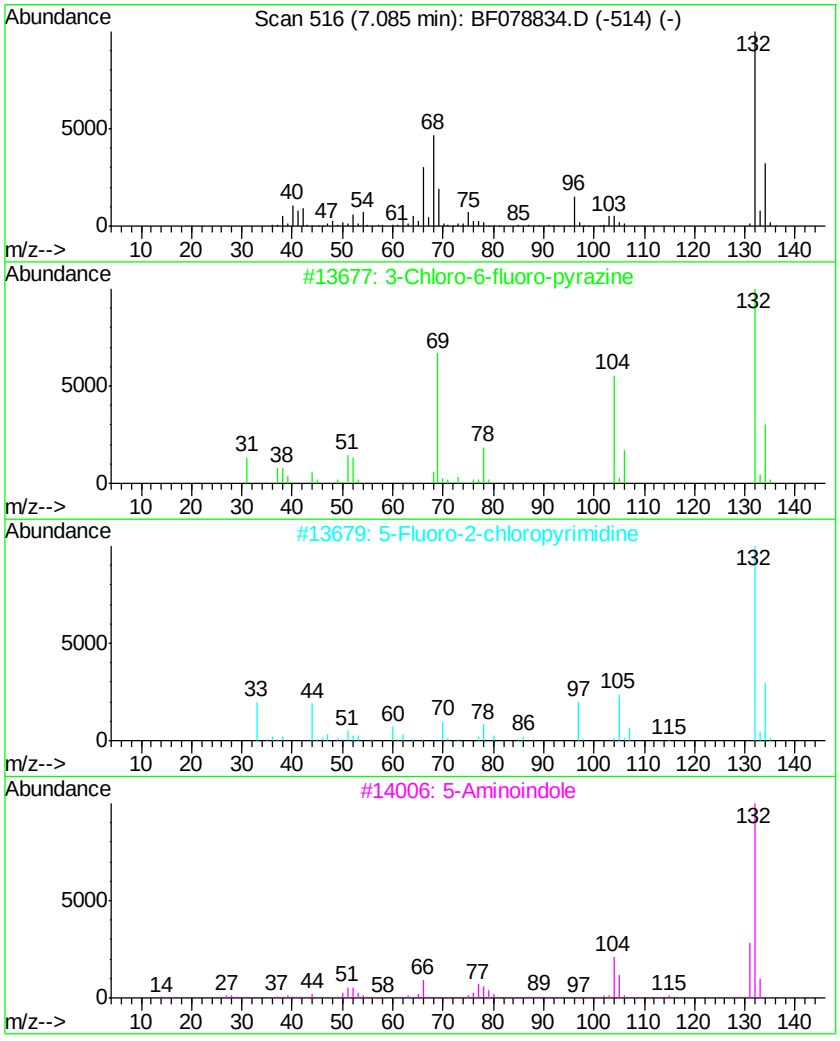
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

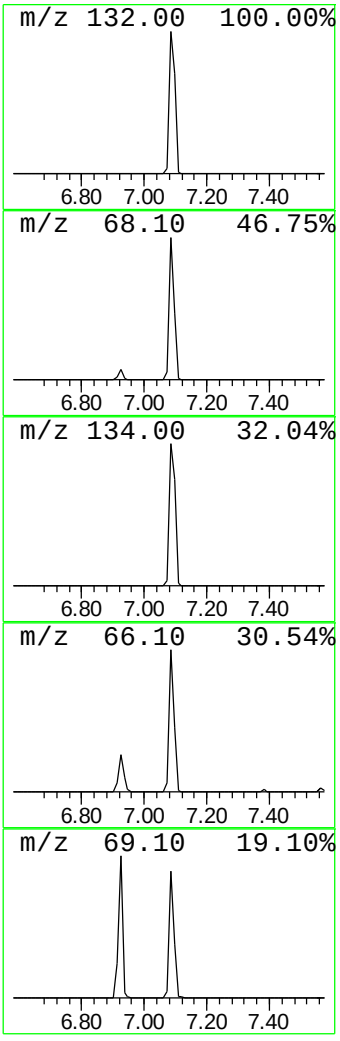
****

Peak Number 8 unknown7.08 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.08	58.23 ng	1209850	1,4-Dichlorobenzene-d4	7.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	1,2,3-Trifluorobenzene	132	C6H3F3	001489-53-8	9





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Sample : G2022-14
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-10-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042815.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

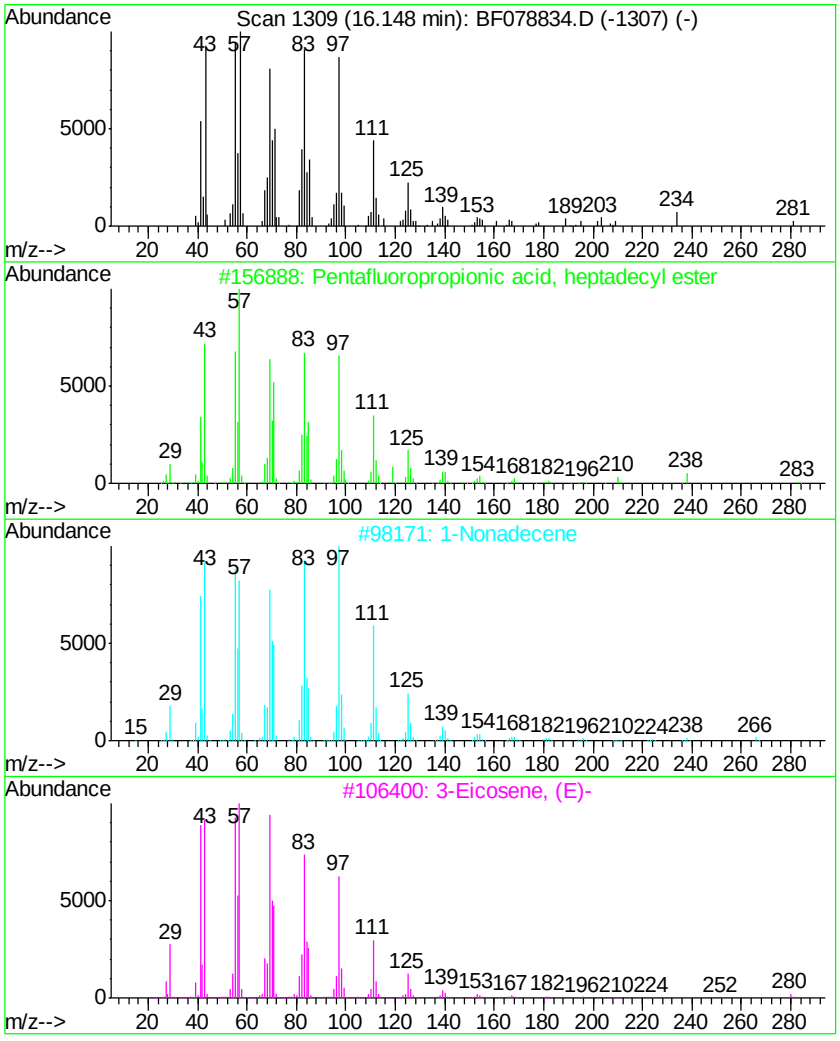
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

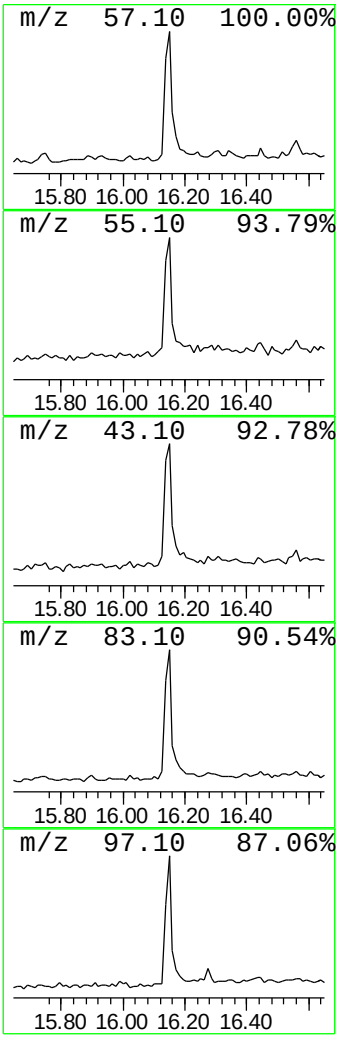
****

Peak Number 11 Pentafluoropropionic acid, ... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.15	4.55 ng	246267	Chrysene-d12	16.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	93
2	1-Nonadecene	266	C19H38	018435-45-5	91
3	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
4	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	90
5	1-Octadecanol	270	C18H38O	000112-92-5	87





Tentatively Identified Compound (LSC) summary

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ClientSampleId : SB-10-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042815.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Cyclopentane, met...	1.28	97.2	ng	2020220	1	7.38	415556	20.0
unknown1.53	1.53	243.5	ng	5059970	1	7.38	415556	20.0
Butane, 2-methoxy...	1.85	10.3	ng	213965	1	7.38	415556	20.0
2-Pentanone, 4-hy...	5.19	7.5	ng	155181	1	7.38	415556	20.0
unknown7.08	7.08	58.2	ng	1209850	1	7.38	415556	20.0
Pentafluoropropio...	16.15	4.5	ng	246267	5	16.27	1083480	20.0