LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF050615\
Data File : BF078964.D
Acq On : 6 May 2015 17:02
Operator : TP/IZ
Sample : G2114-14 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GRID-5(6-12)

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	1.255	3	6	8	rVB	523300	724101	17.00%	3.198%
2	1.484	24	26	29	rVB	1579121	2171683	51.00%	9.592%
3	1.633	36	39	42	rVB	426118	589830	13.85%	2.605%
4	1.770	49	51	53	rBV	115207	152621	3.58%	0.674%
5	1.815	53	55	60	rVB	96912	151345	3.55%	0.668%
6	1.895	60	62	86	rVB	2500994	4258525	100.00%	18.810%
7	5.153	343	347	352	rBV	49730	61765	1.45%	0.273%
8	5.644	387	390	393	rBV	556743	574836	13.50%	2.539%
9	6.890	497	499	502	rBV	463644	602338	14.14%	2.661%
10	7.050	511	513	516	rBV	488244	619883	14.56%	2.738%
11	7.347	537	539	541	rBV	499252	431635	10.14%	1.907%
12	7.530	553	555	558	rVB	464804	466675	10.96%	2.061%
13	8.033	597	599	602	rBV	417995	368069	8.64%	1.626%
14	8.925	674	677	679	rBV	692999	606490	14.24%	2.679%
15	10.273	792	795	797	rBV	580376	717683	16.85%	3.170%
16	11.096	865	867	870	rBV	568916	668576	15.70%	2.953%
17	11.999	944	946	949	rVB	72220	68028	1.60%	0.300%
18	12.079	950	953	956	rBV	481390	456760	10.73%	2.017%
19	12.948	1026	1029	1030	rBV	787726	729942	17.14%	3.224%
20	12.971	1030	1031	1034	rVV	199378	234781	5.51%	1.037%
21	13.039	1034	1037	1039	rVB	63745	59901	1.41%	0.265%
22	13.611	1085	1087	1089	rVB	46551	42608	1.00%	0.188%
23	13.714	1094	1096	1097	rBV	34385	43248	1.02%	0.191%
24	13.954	1115	1117	1121	rBV2	28308	48878	1.15%	0.216%
25	14.457	1158	1161	1164	rBV	532618	512330	12.03%	2.263%
26	14.731	1182	1185	1188	rVV	338333	514709	12.09%	2.273%
27	14.800	1189	1191	1197	rVV	147748	240999	5.66%	1.064%
28	14.937	1201	1203	1206	rVV	633861	853213	20.04%	3.769%
29	15.280	1231	1233	1235	rBV	54453	63879	1.50%	0.282%
30	15.794	1275	1278	1281	rBV	55290	75761	1.78%	0.335%
31	15.931	1287	1290	1292	rVV	52030	88307	2.07%	0.390%
32	15.977	1292	1294	1297	rVV3	50452	103967	2.44%	0.459%
33	16.057	1299	1301	1304	rVV2	51233	70024	1.64%	0.309%
34	16.125	1304	1307	1313	rVV4	44856	90472	2.12%	0.400%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF050615\
Data File : BF078964.D
Acq On : 6 May 2015 17:02
Operator : TP/IZ
Sample : G2114-14 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GRID-5(6-12)

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

35	16.263	1315	1319	1320	rVV2	797639	1222114	28.70%	5.398%
36	16.297	1320	1322	1325	rVV	953267	1169430	27.46%	5.165%
37	16.685	1353	1356	1358	rBV3	23160	53804	1.26%	0.238%
38	16.731	1358	1360	1361	rVV	38762	68179	1.60%	0.301%
39	16.777	1362	1364	1366	rVV	51827	71658	1.68%	0.317%
40	17.394	1415	1418	1423	rVB3	31310	74945	1.76%	0.331%
41	17.611	1434	1437	1444	rBV	211095	558682	13.12%	2.468%
42	17.737	1446	1448	1450	rVB	47382	61862	1.45%	0.273%
43	17.943	1464	1466	1470	rVB	134815	180503	4.24%	0.797%
44	18.011	1470	1472	1475	rBV	189145	211770	4.97%	0.935%
45	18.080	1475	1478	1480	rBV	762151	950904	22.33%	4.200%
46	19.154	1569	1572	1575	rBV5	33714	99722	2.34%	0.440%
47	19.589	1607	1610	1617	rVB2	109299	279623	6.57%	1.235%
48	20.034	1645	1649	1654	rVB	77213	172843	4.06%	0.763%

Sum of corrected areas: 22639901

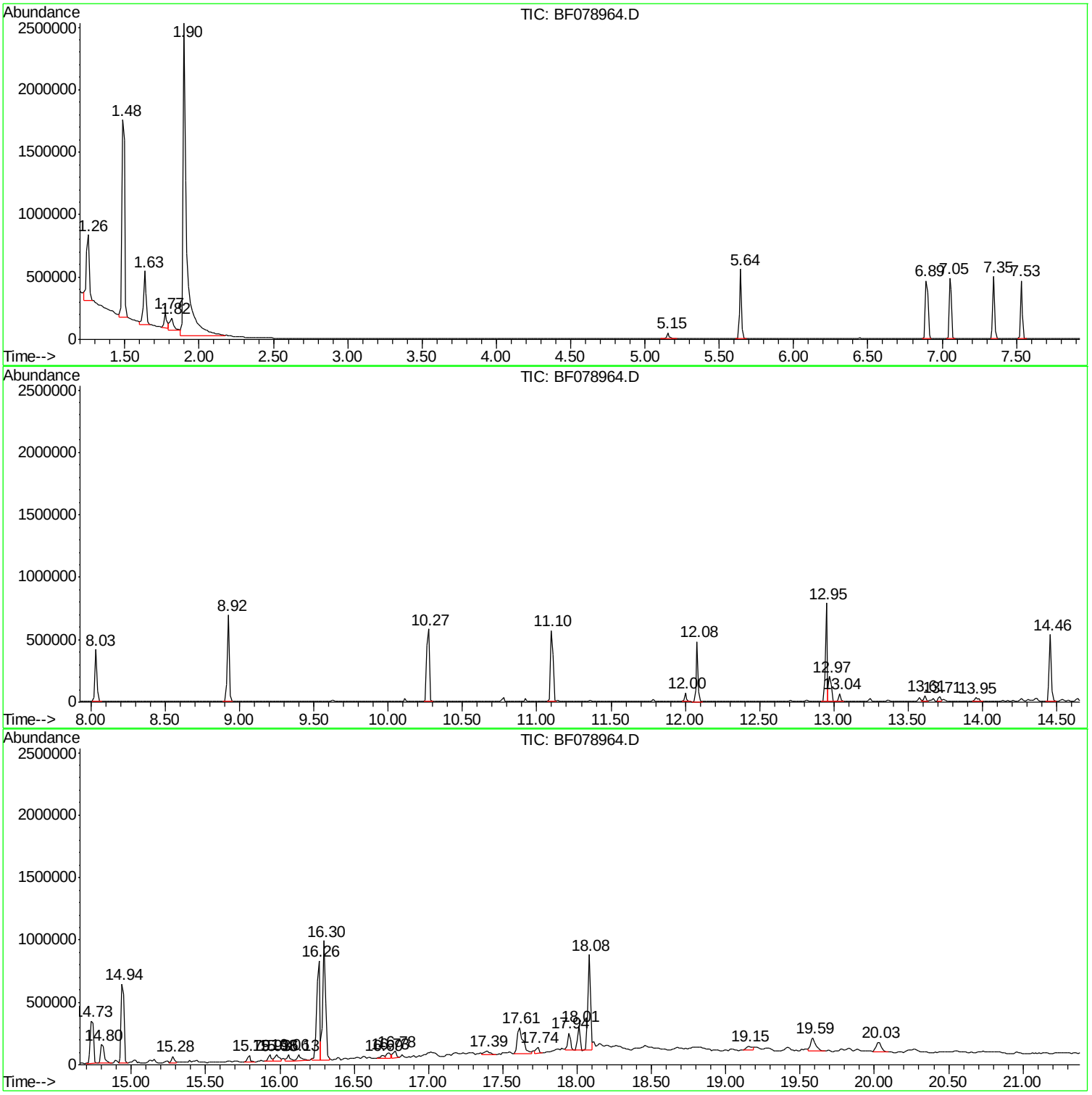
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF050615\
Data File : BF078964.D
Acq On : 6 May 2015 17:02
Operator : TP/IZ
Sample : G2114-14 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GRID-5(6-12)

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF050615\
Data File : BF078964.D
Acq On : 6 May 2015 17:02
Operator : TP/IZ
Sample : G2114-14 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GRID-5(6-12)

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

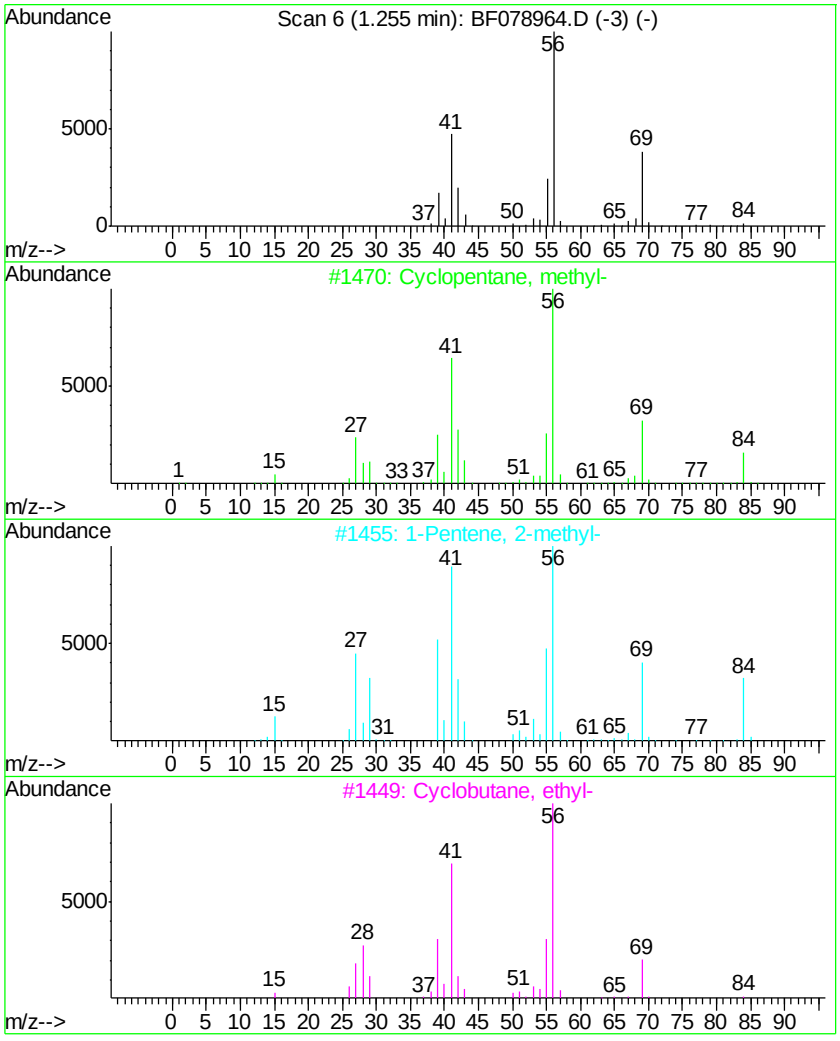
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

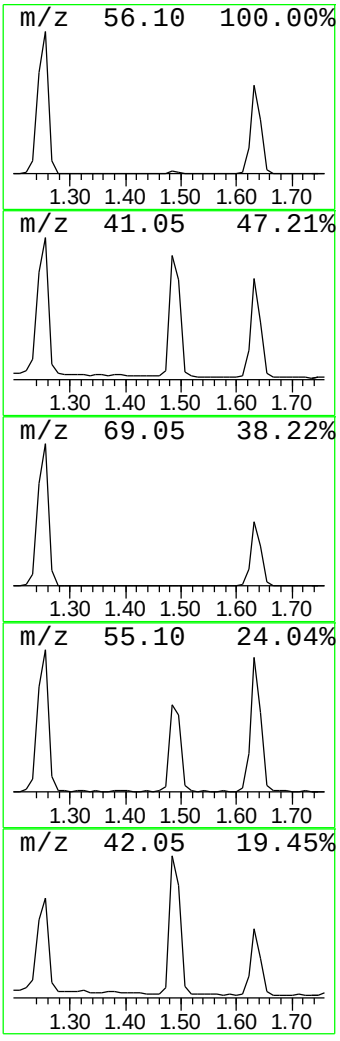
****

Peak Number 1 Cyclopentane, methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.26	33.55 ng	724101	1,4-Dichlorobenzene-d4	7.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	90
2	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	40
3	Cyclobutane, ethyl-	84	C6H12	004806-61-5	10
4	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	9
5	Cyclopropane, propyl-	84	C6H12	002415-72-7	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF050615\
Data File : BF078964.D
Acq On : 6 May 2015 17:02
Operator : TP/IZ
Sample : G2114-14 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GRID-5(6-12)

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

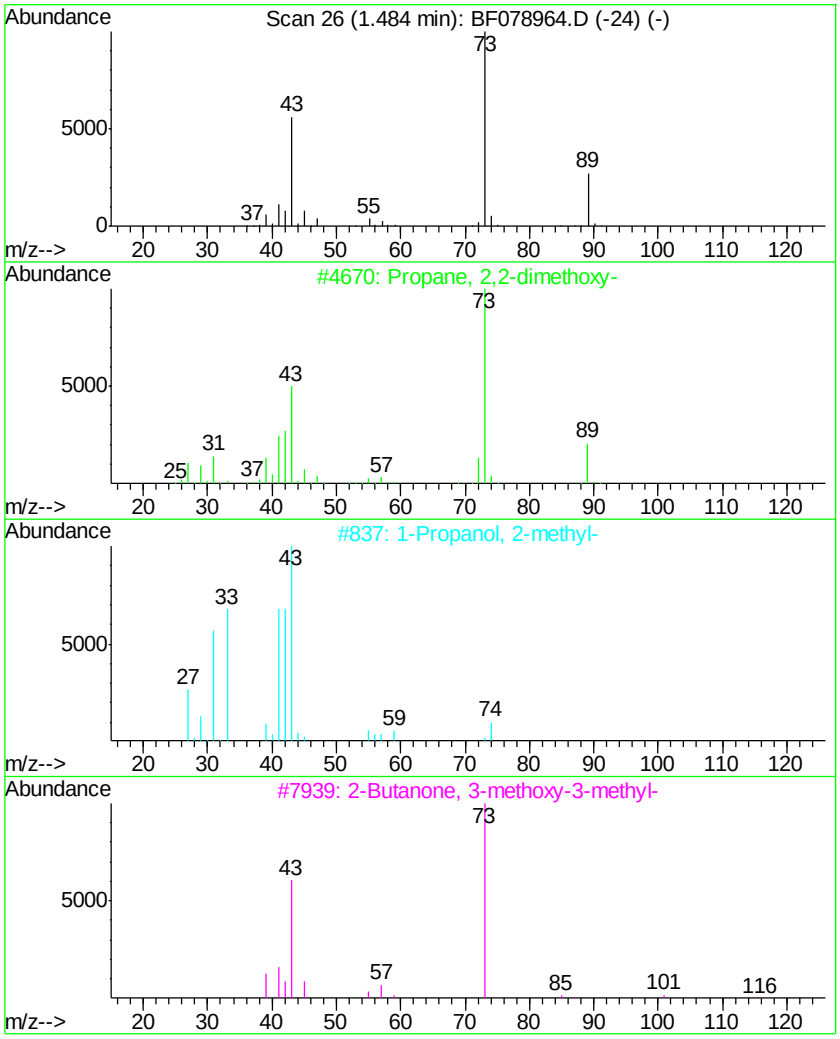
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

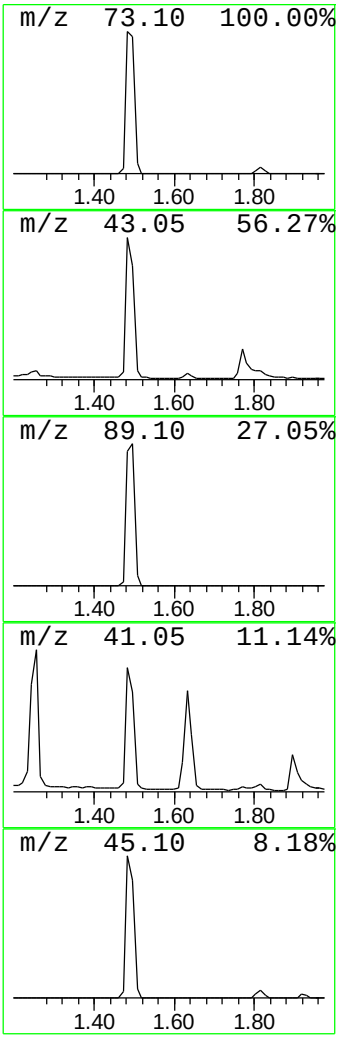
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.48	100.63 ng	2171680	1,4-Dichlorobenzene-d4	7.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	72
2	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9
3	2-Butanone, 3-methoxy-3-methyl-	116	C6H12O2	036687-98-6	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





Data Path : Z:\HPCHEM1\BNA F\DATA\BF050615\
Data File : BF078964.D
Acq On : 6 May 2015 17:02
Operator : TP/IZ
Sample : G2114-14 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GRID-5(6-12)

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

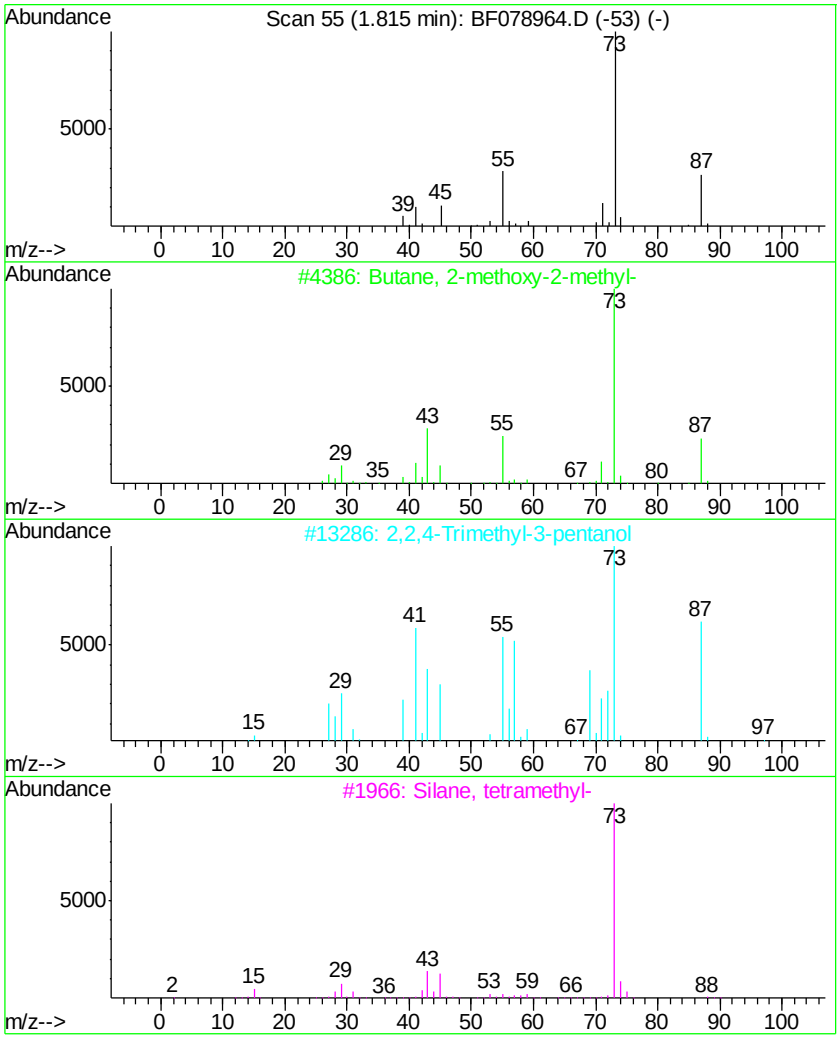
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

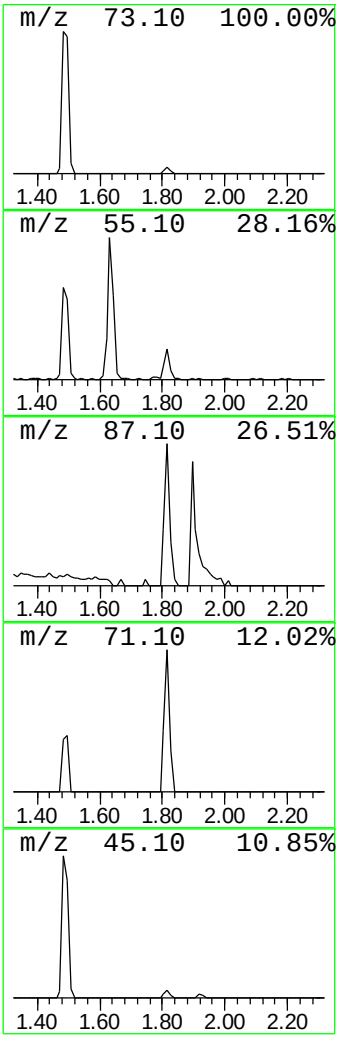
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.82	7.01 ng	151345	1,4-Dichlorobenzene-d4	7.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	Silane, tetramethyl-	88	C4H12Si	000075-76-3	32
4	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF050615\
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Sample : G2114-14 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GRID-5(6-12)

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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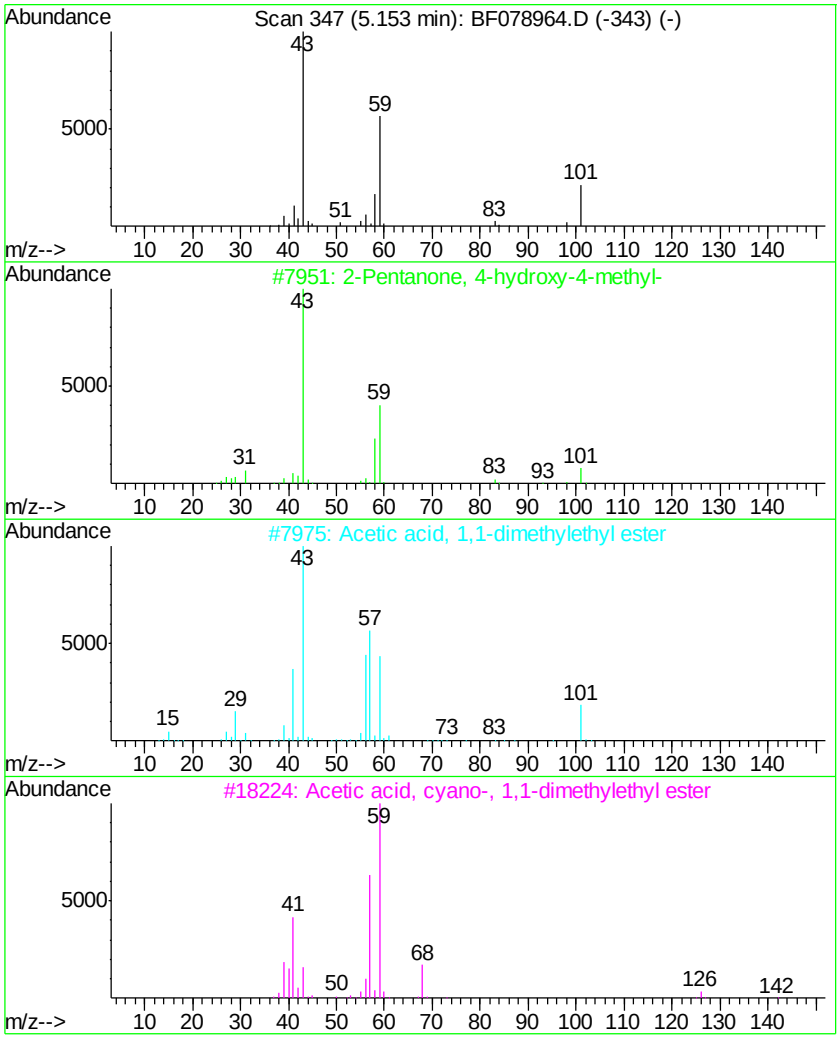
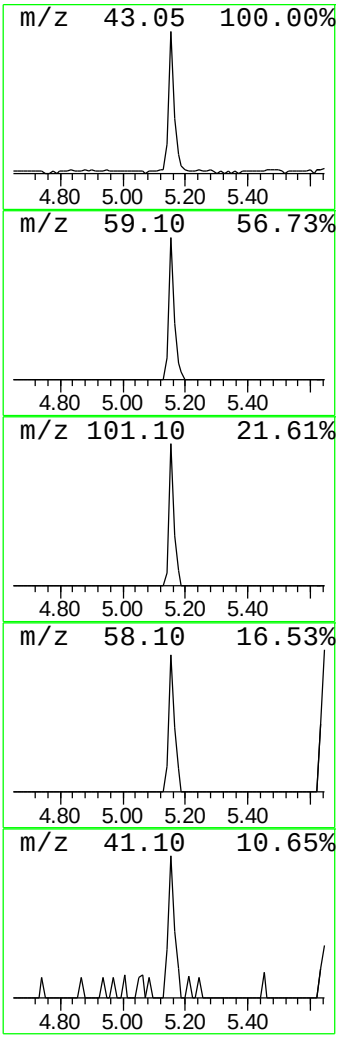
Peak Number 7 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.15	2.86 ng	61765	1,4-Dichlorobenzene-d4	7.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF050615\
Data File : BF078964.D
Acq On : 6 May 2015 17:02
Operator : TP/IZ
Sample : G2114-14 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GRID-5(6-12)

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

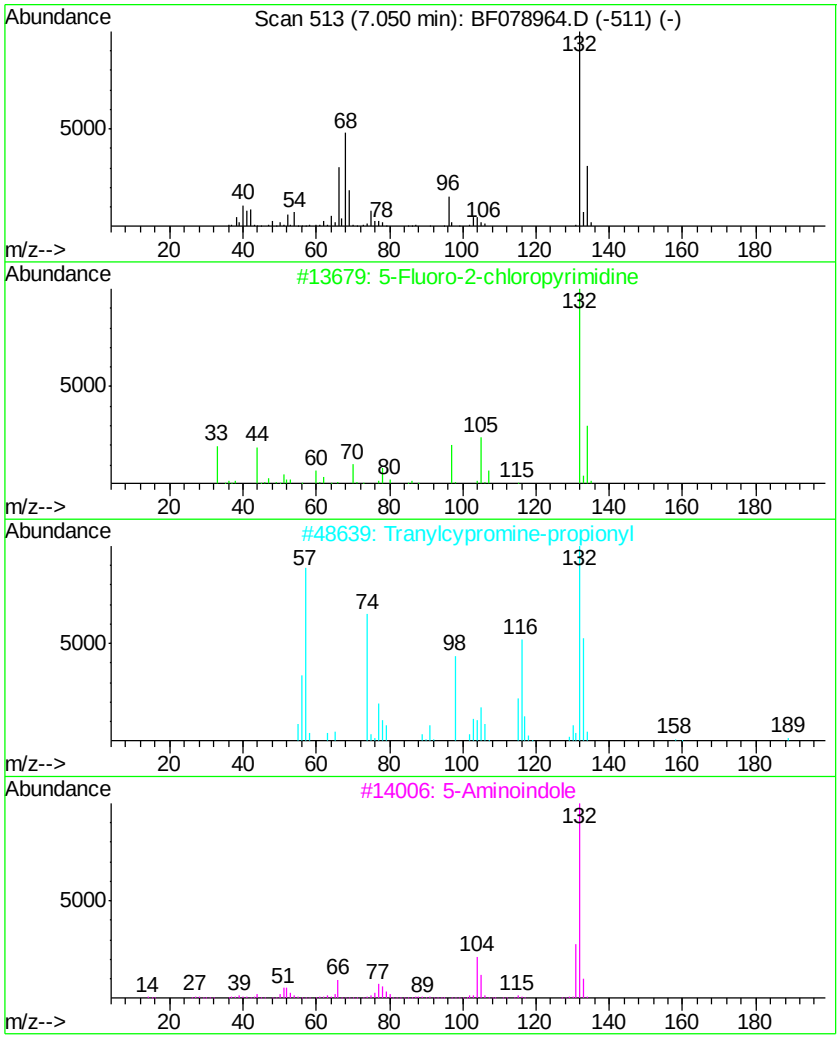
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

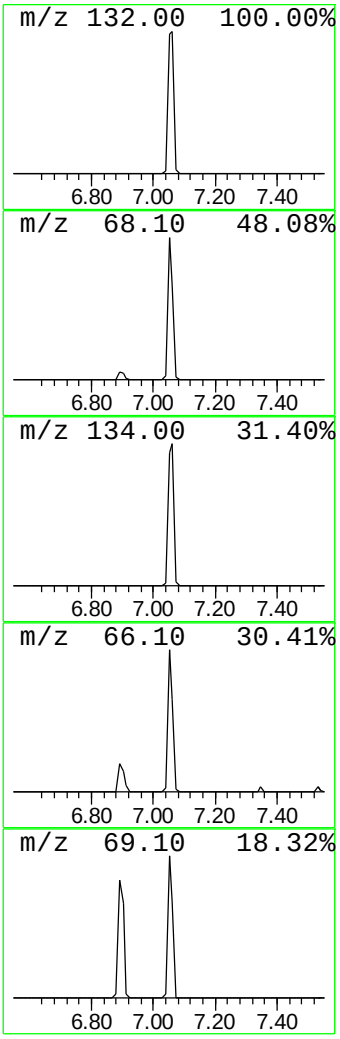
****

Peak Number 8 unknown7.05 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.05	28.72 ng	619883	1,4-Dichlorobenzene-d4	7.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	5-Aminoindole	132	C8H8N2	005192-03-0	10
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF050615\
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Operator : TP/IZ
Sample : G2114-14 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GRID-5(6-12)

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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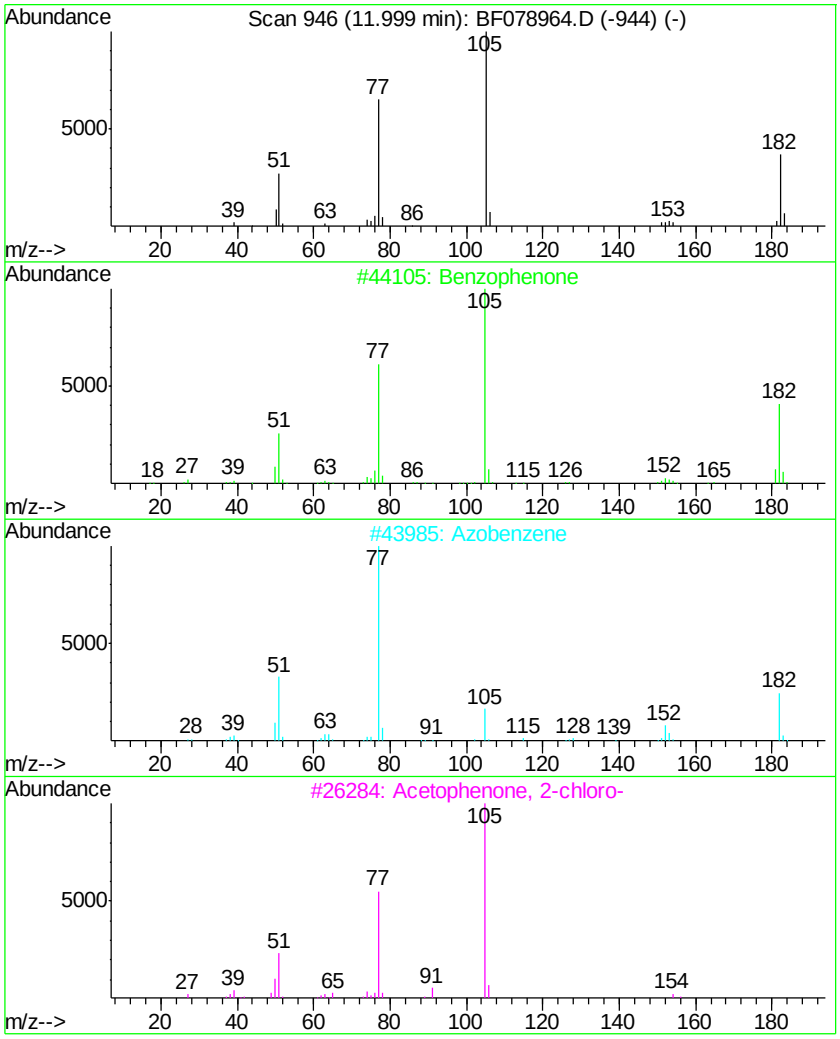
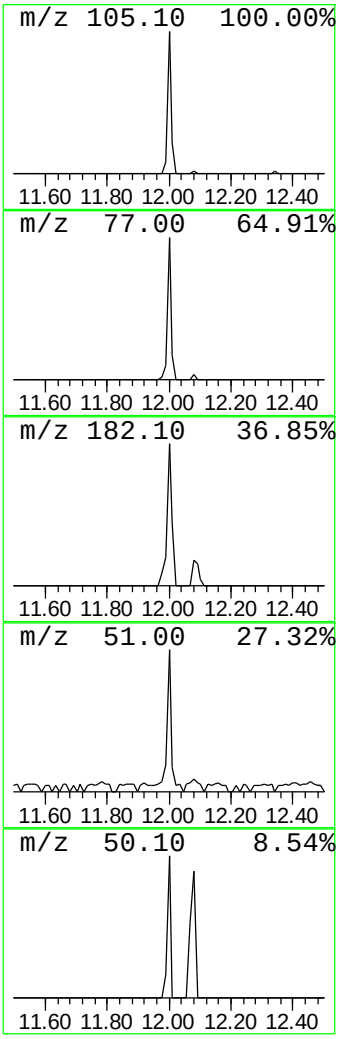
Peak Number 10 Benzophenone Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.00	2.04 ng	68028	Acenaphthene-d10	11.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	94
2	Azobenzene	182	C12H10N2	000103-33-3	59
3	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	58
4	Ethanedione, diphenyl-	210	C14H10O2	000134-81-6	53
5	4-Acetylphenylbenzoate	240	C15H12O3	001523-18-8	53





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Acq On : 6 May 2015 17:02
Operator : TP/IZ
Sample : G2114-14 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GRID-5(6-12)

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

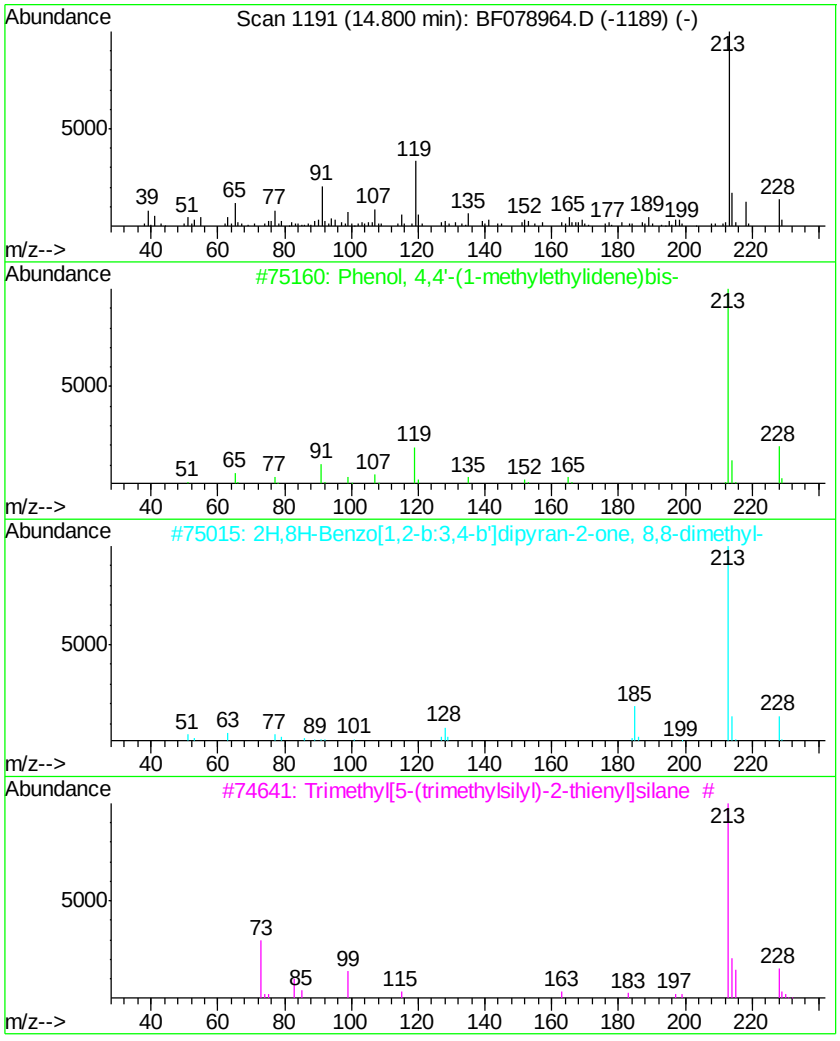
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

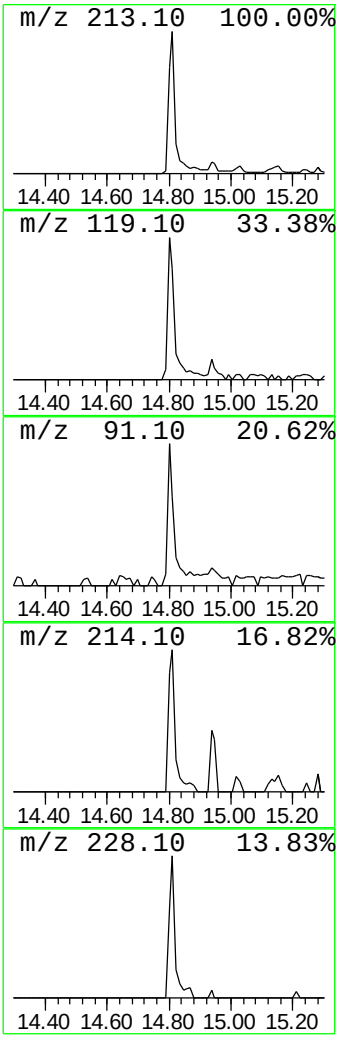
****

Peak Number 11 Phenol, 4,4'-(1-methylethyl... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.80	3.94 ng	240999	Chrysene-d12	16.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	96
2	2H,8H-Benzo[1,2-b:3,4-b']dipyran...	228	C14H12O3	000523-59-1	58
3	Trimethyl[5-(trimethylsilyl)-2-t...	228	C10H20SSi2	017906-71-7	53
4	Carbanilic acid, p-phenyl-	213	C13H11NO2	004474-53-7	52
5	2,4(1H,3H)-Pyrimidinedione, 1,3-...	228	C9H16N2O3Si	089447-84-7	42





Data Path : Z:\HPCHEM1\BNA F\DATA\BF050615\
Data File : BF078964.D
Acq On : 6 May 2015 17:02
Operator : TP/IZ
Sample : G2114-14 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GRID-5(6-12)

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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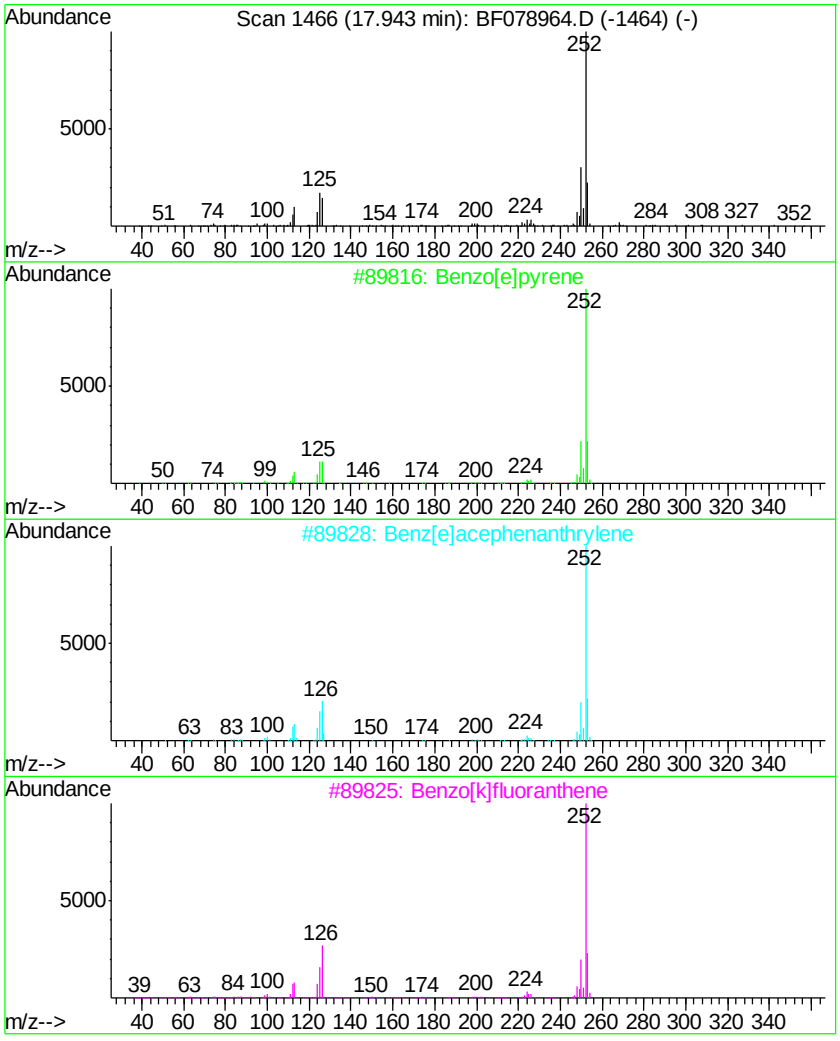
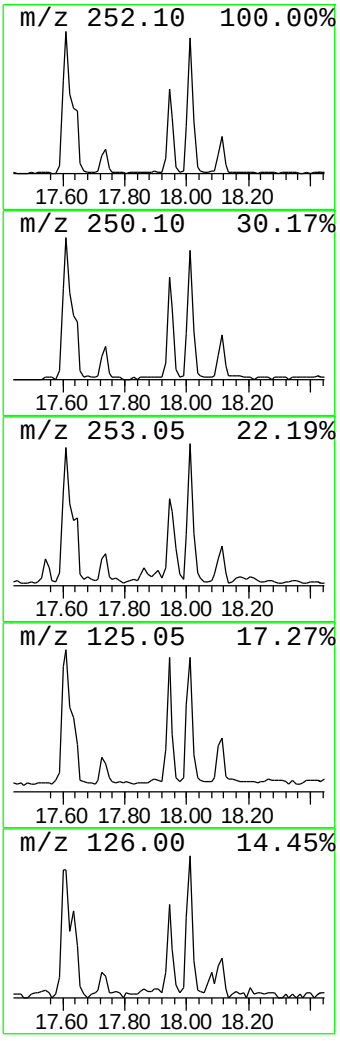
Peak Number 12 Benzo[e]pyrene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.94	3.80 ng	180503	Perylene-d12	18.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	97
2	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	96
3	Benzo[k]fluoranthene	252	C20H12	000207-08-9	90
4	Benzo[a]pyrene	252	C20H12	000050-32-8	87
5	Perylene	252	C20H12	000198-55-0	81





Data Path : Z:\HPCHEM1\BNA F\DATA\BF050615\
Data File : BF078964.D
Acq On : 6 May 2015 17:02
Operator : TP/IZ
Sample : G2114-14 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GRID-5(6-12)

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

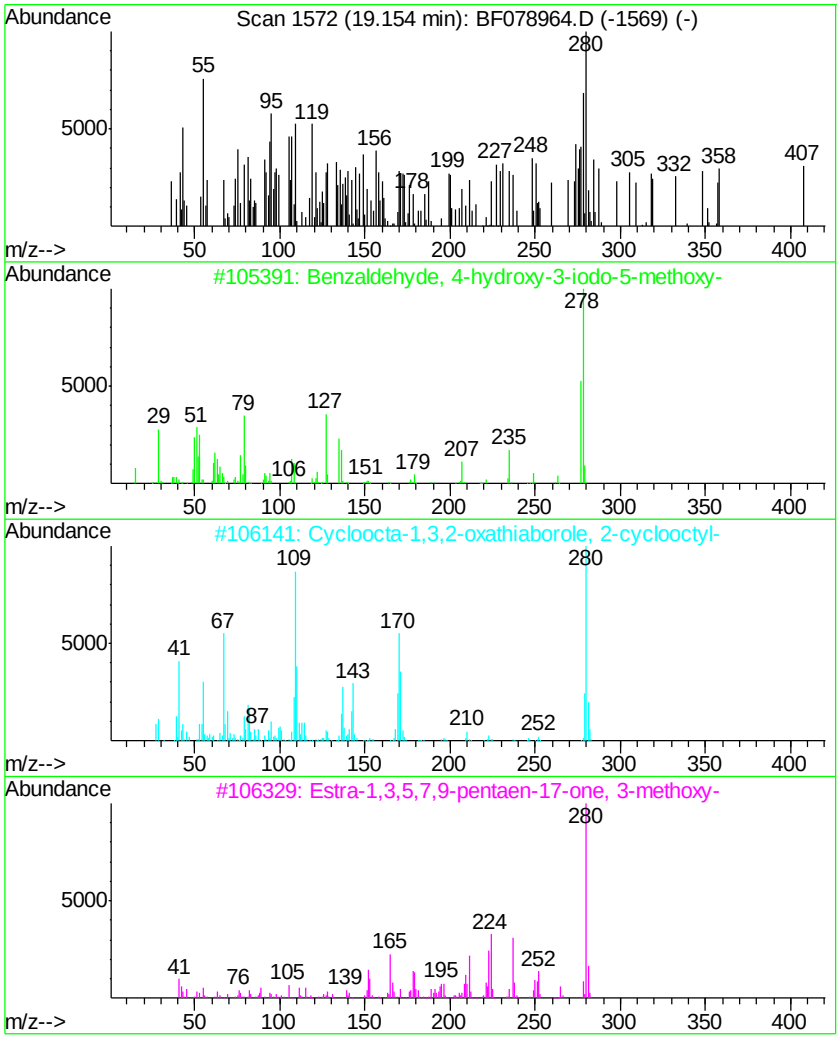
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

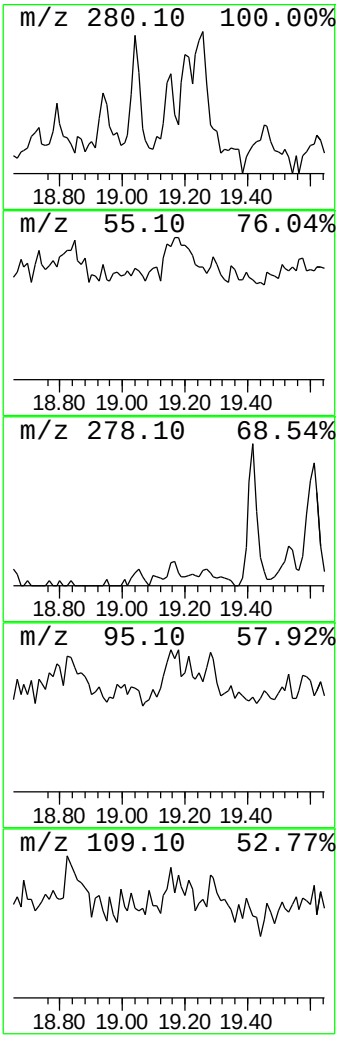
****

Peak Number 13 unknown19.15 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.15	2.10 ng	99722	Perylene-d12	18.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzaldehyde, 4-hydroxy-3-iodo-5...	278	C8H7IO3	005438-36-8	25
2	Cycloocta-1,3,2-oxathiaborole, 2...	280	C16H29BOS	1000161-43-2	25
3	Estra-1,3,5,7,9-pentaen-17-one, ...	280	C19H20O2	003907-67-3	25
4	3,7-Dibromotropolone	278	C7H4Br2O2	004636-41-3	18
5	Pteridin-4-ol, 6,7-bis(2-furyl)-	280	C14H8N4O3	313996-29-1	15





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050615\
Data File : BF078964.D
Acq On : 6 May 2015 17:02
Operator : TP/IZ
Sample : G2114-14 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GRID-5(6-12)

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Cyclopentane, met...	1.26	33.5	ng	724101	1	7.35	431635	20.0
Propane, 2,2-dime...	1.48	100.6	ng	2171680	1	7.35	431635	20.0
Butane, 2-methoxy...	1.82	7.0	ng	151345	1	7.35	431635	20.0
2-Pentanone, 4-hy...	5.15	2.9	ng	61765	1	7.35	431635	20.0
unknown7.05	7.05	28.7	ng	619883	1	7.35	431635	20.0
Benzophenone	12.00	2.0	ng	68028	3	11.10	668576	20.0
Phenol, 4,4'-(1-m...	14.80	3.9	ng	240999	5	16.26	1222110	20.0
Benzo[e]pyrene	17.94	3.8	ng	180503	6	18.08	950904	20.0
unknown19.15	19.15	2.1	ng	99722	6	18.08	950904	20.0