LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032415\
Data File : BF077937.D
Acq On : 25 Mar 2015 5:32
Operator : TP/IZ
Sample : G1613-09
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-5-1

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-BF031115.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	1.047	11	14	17	rVB	552048	824490	35.76%	5.131%
2	1.264	31	33	36	rVB	2202413	2305880	100.00%	14.351%
3	1.390	41	44	47	rVB	530173	763894	33.13%	4.754%
4	1.550	56	58	64	rVB	64719	87256	3.78%	0.543%
5	1.653	65	67	75	rVV	71658	122096	5.29%	0.760%
6	1.767	75	77	96	rVB	603346	1047623	45.43%	6.520%
7	4.864	346	348	356	rVB	86614	108322	4.70%	0.674%
8	5.401	393	395	398	rBV	761507	867101	37.60%	5.397%
9	6.693	506	508	511	rBV	784701	884832	38.37%	5.507%
10	6.830	518	520	523	rBV	1085567	978208	42.42%	6.088%
11	7.116	543	545	548	rBV	285774	257992	11.19%	1.606%
12	7.299	559	561	564	rBV	656829	738738	32.04%	4.598%
13	7.813	603	606	608	rBV	665496	586114	25.42%	3.648%
14	8.693	681	683	686	rBV	421571	361665	15.68%	2.251%
15	10.042	799	801	803	rBV	1507376	1290238	55.95%	8.030%
16	10.545	843	845	848	rBV	24154	29508	1.28%	0.184%
17	10.865	871	873	875	rBV	436852	414550	17.98%	2.580%
18	11.848	956	959	961	rBV	505982	713911	30.96%	4.443%
19	12.042	974	976	981	rVB	18080	23450	1.02%	0.146%
20	12.705	1031	1034	1036	rBV	342244	440485	19.10%	2.741%
21	14.694	1205	1208	1211	rBV	1500012	1471403	63.81%	9.158%
22	15.894	1310	1313	1319	rBV	45669	111204	4.82%	0.692%
23	15.997	1319	1322	1324	rBV	435014	504991	21.90%	3.143%
24	16.168	1334	1337	1340	rBV	43845	47792	2.07%	0.297%
25	16.671	1378	1381	1384	rBV2	33596	45972	1.99%	0.286%
26	17.803	1477	1480	1483	rBV	413042	544987	23.63%	3.392%
27	18.900	1574	1576	1584	rVB	23075	48263	2.09%	0.300%
28	19.369	1614	1617	1622	rBV	177733	322386	13.98%	2.006%
29	19.677	1641	1644	1651	rVB6	27717	61042	2.65%	0.380%
30	20.123	1680	1683	1689	rVB7	27553	62929	2.73%	0.392%

Sum of corrected areas: 16067322

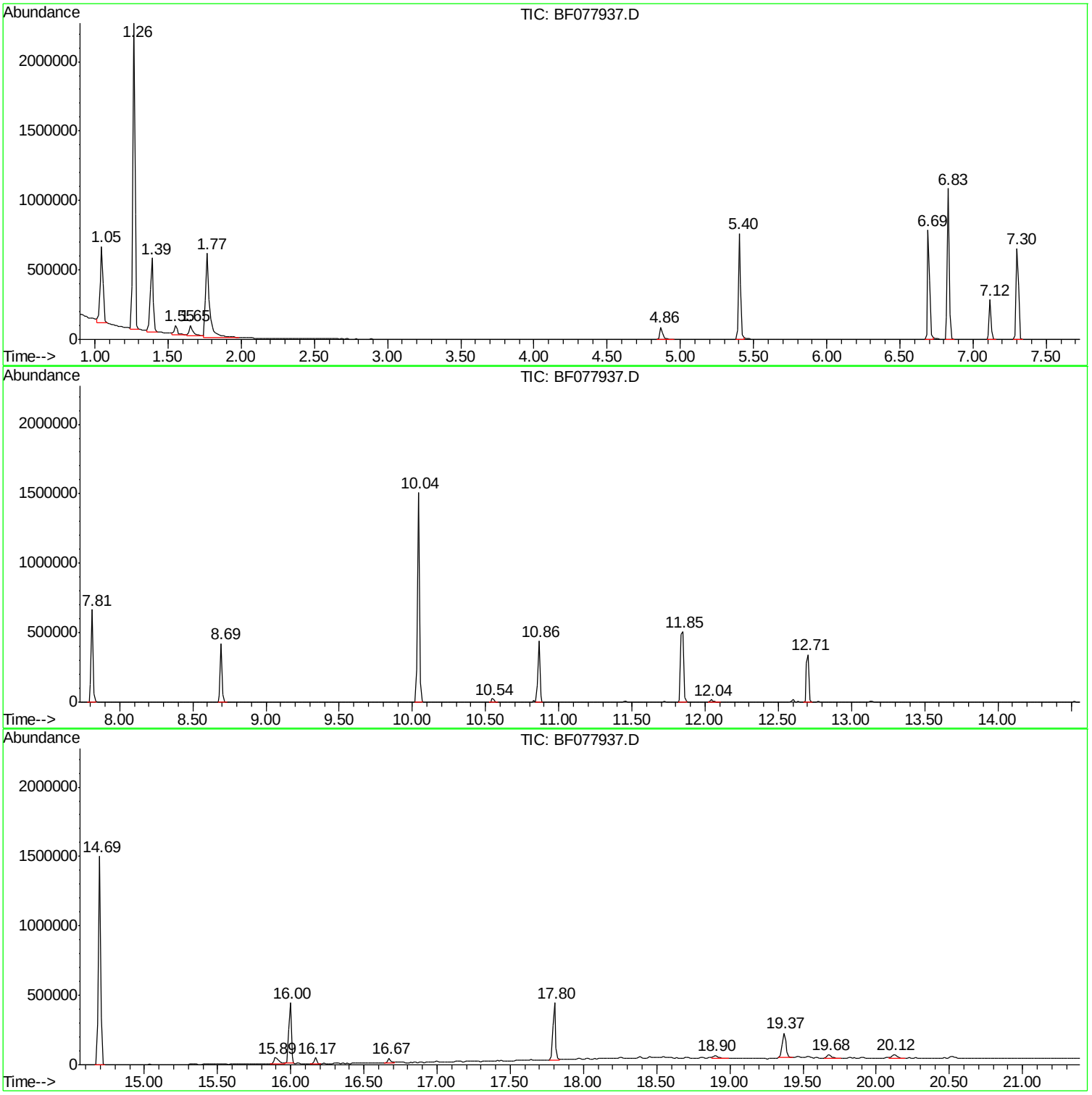
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032415\
Data File : BF077937.D
Acq On : 25 Mar 2015 5:32
Operator : TP/IZ
Sample : G1613-09
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-5-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031115.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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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

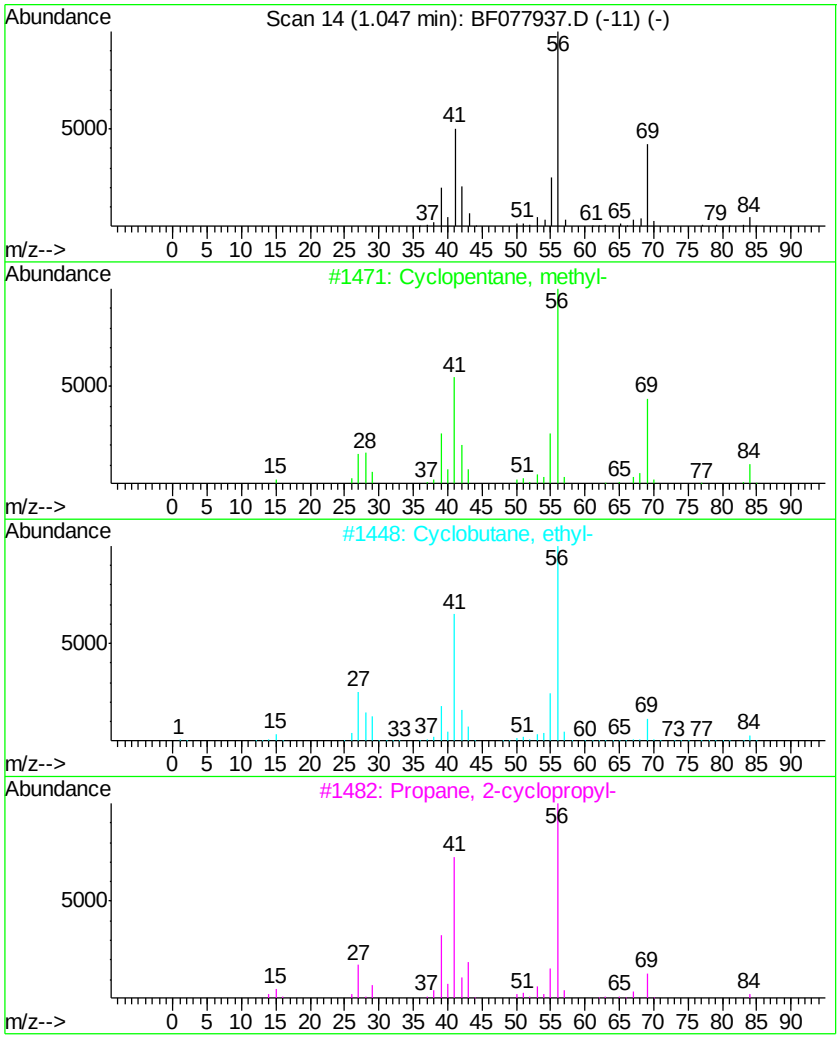
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

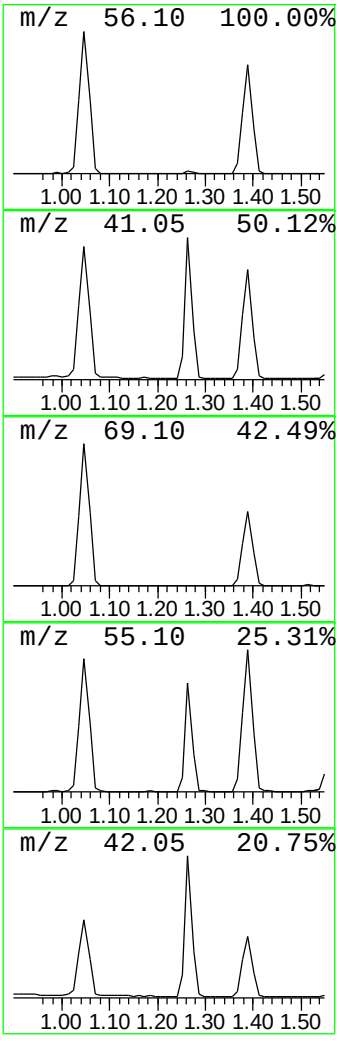
****

Peak Number 1 Cyclopentane, methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.05	63.92 ng	824490	1,4-Dichlorobenzene-d4	7.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	91
2	Cyclobutane, ethyl-	84	C6H12	004806-61-5	80
3	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	64
4	Cyclopropane, propyl-	84	C6H12	002415-72-7	40
5	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	39





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Data File : BF077937.D
Acq On : 25 Mar 2015 5:32
Operator : TP/IZ
Sample : G1613-09
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-5-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

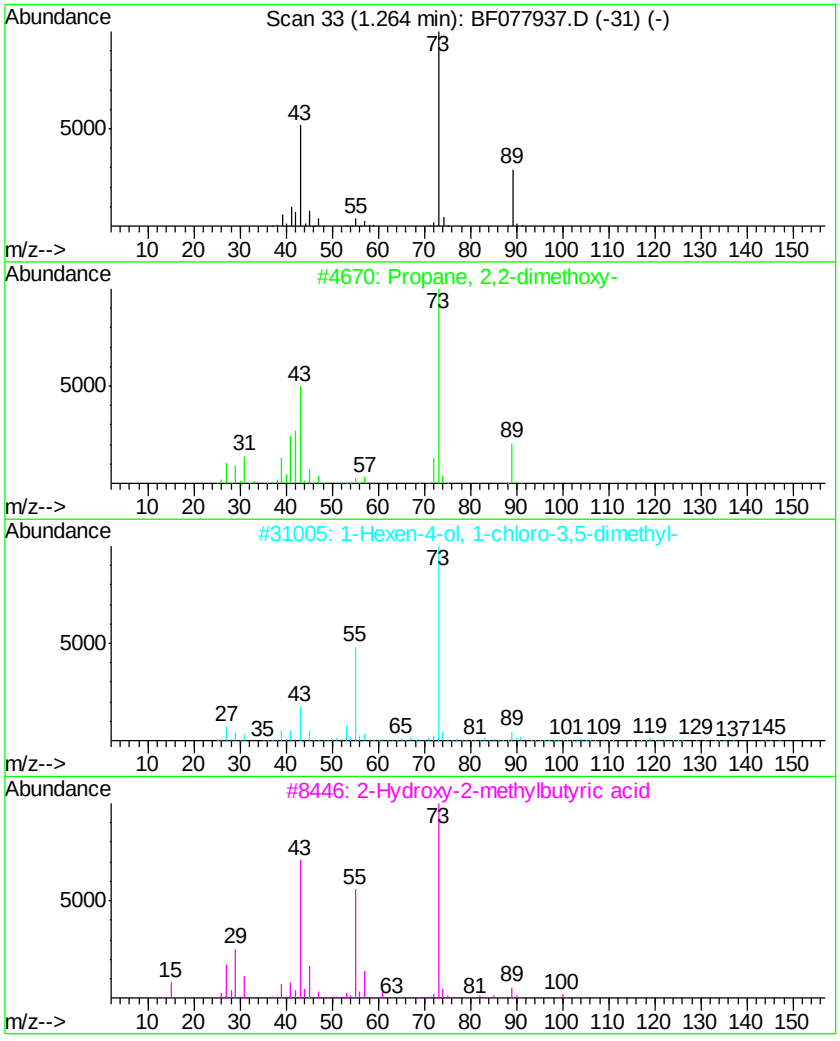
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

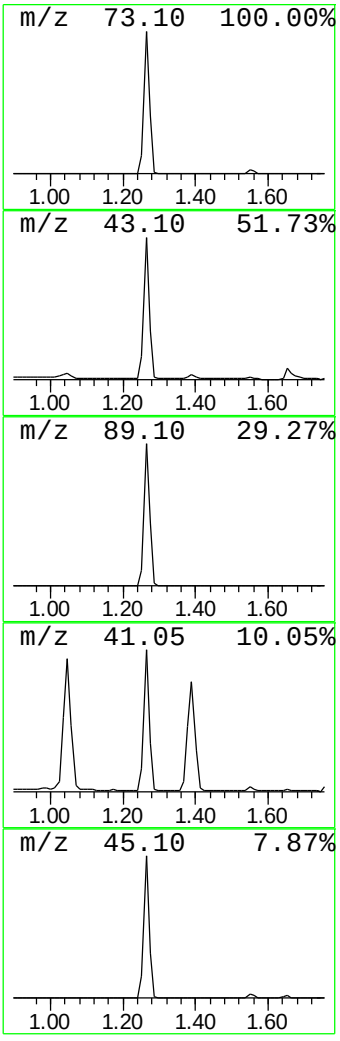
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.26	178.76 ng	2305880	1,4-Dichlorobenzene-d4	7.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	56
2	1-Hexen-4-ol, 1-chloro-3,5-dimet...	162	C8H15ClO	100244-09-5	9
3	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9
4	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	9
5	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9





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Sample : G1613-09
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-5-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

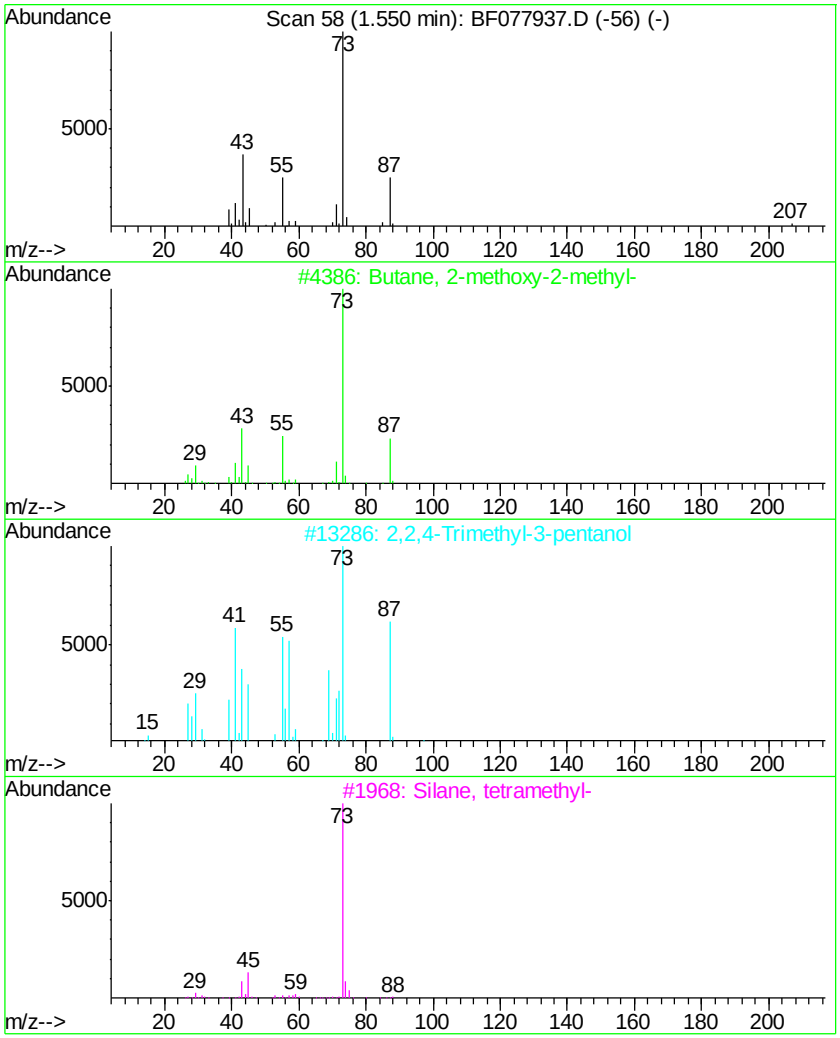
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

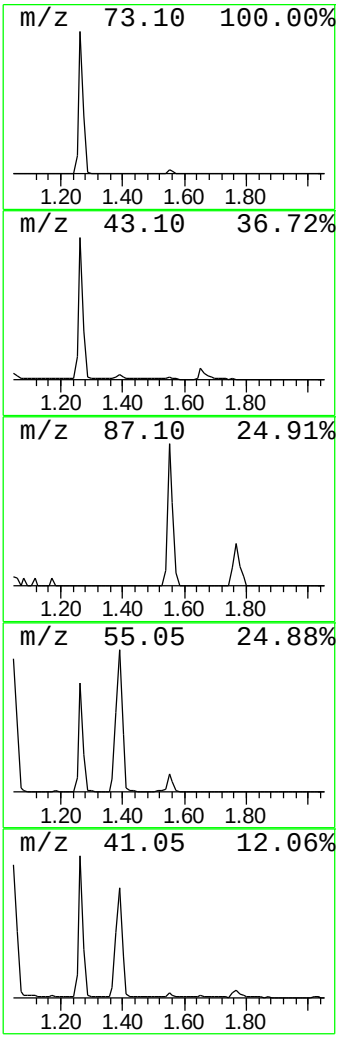
****

Peak Number 4 Butane, 2-methoxy-2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.55	6.76 ng	87256	1,4-Dichlorobenzene-d4	7.12

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	10
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





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Sample : G1613-09
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-5-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

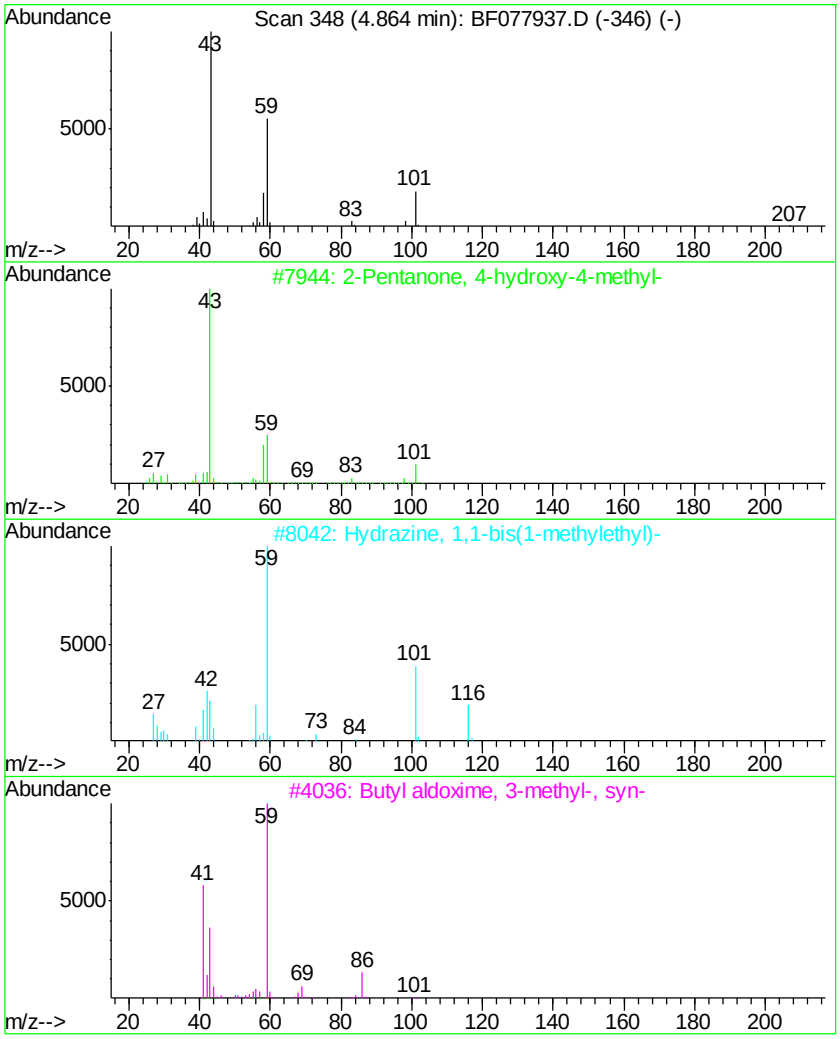
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

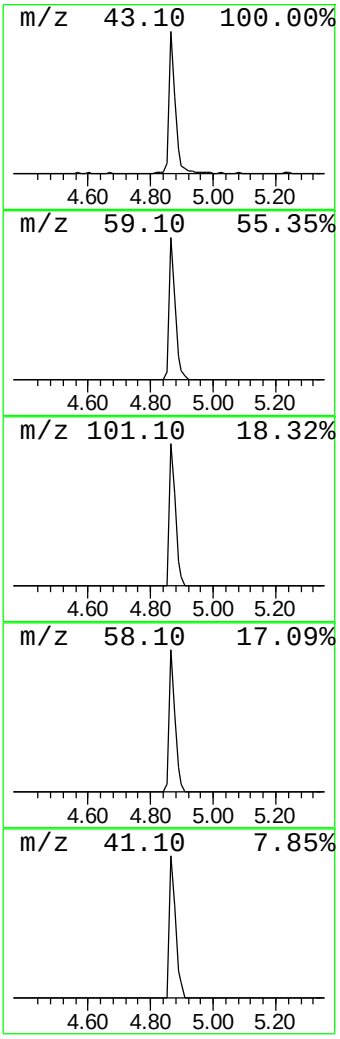
****

Peak Number 7 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.86	8.40 ng	108322	1,4-Dichlorobenzene-d4	7.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	38
3	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	23
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





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Sample : G1613-09
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-5-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

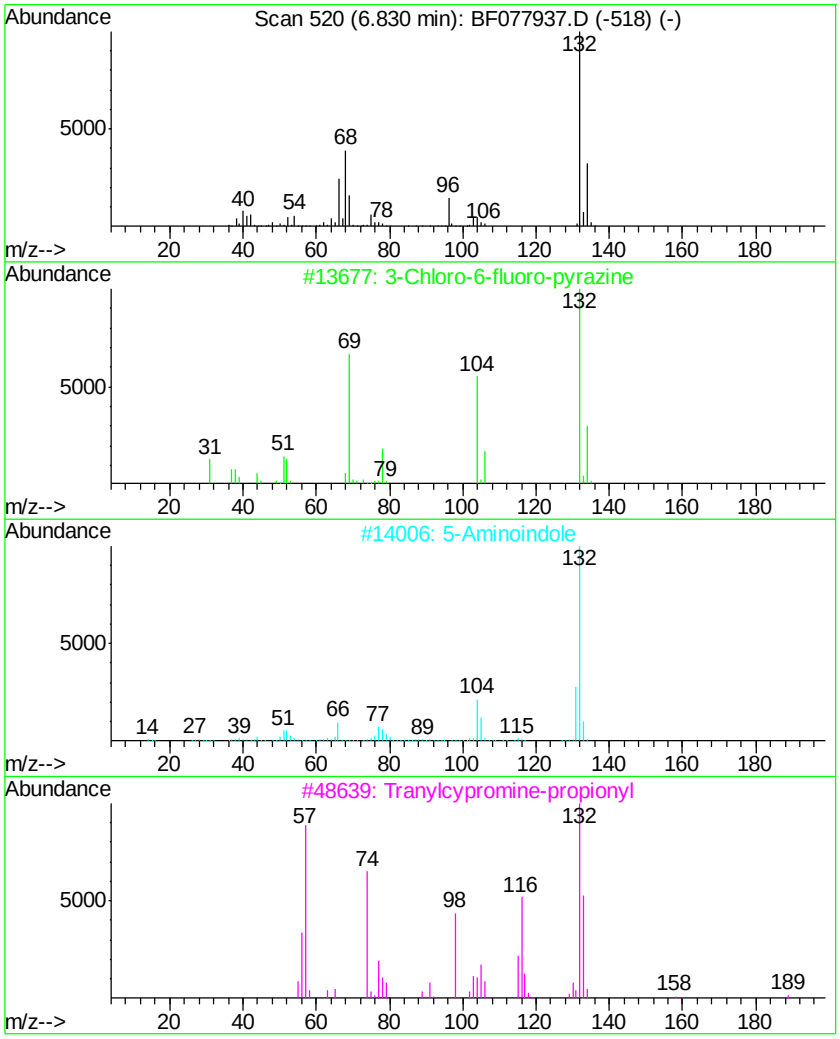
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

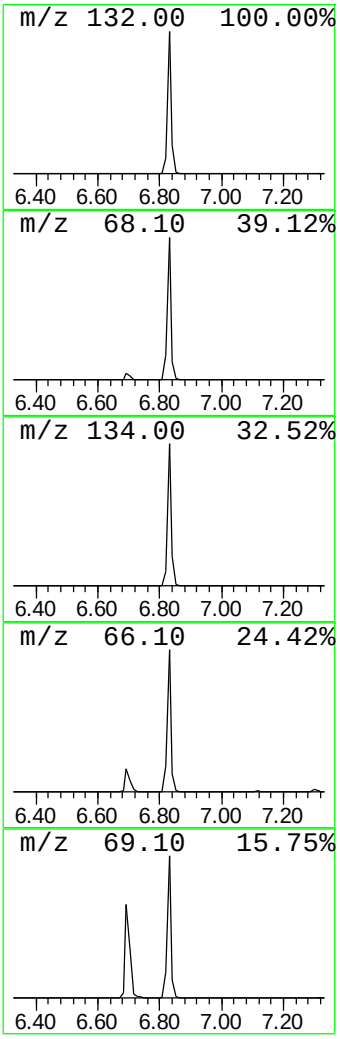
****

Peak Number 8 unknown6.83 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.83	75.83 ng	978208	1,4-Dichlorobenzene-d4	7.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9





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Instrument : BNA_F
ClientSampleId : SB-5-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

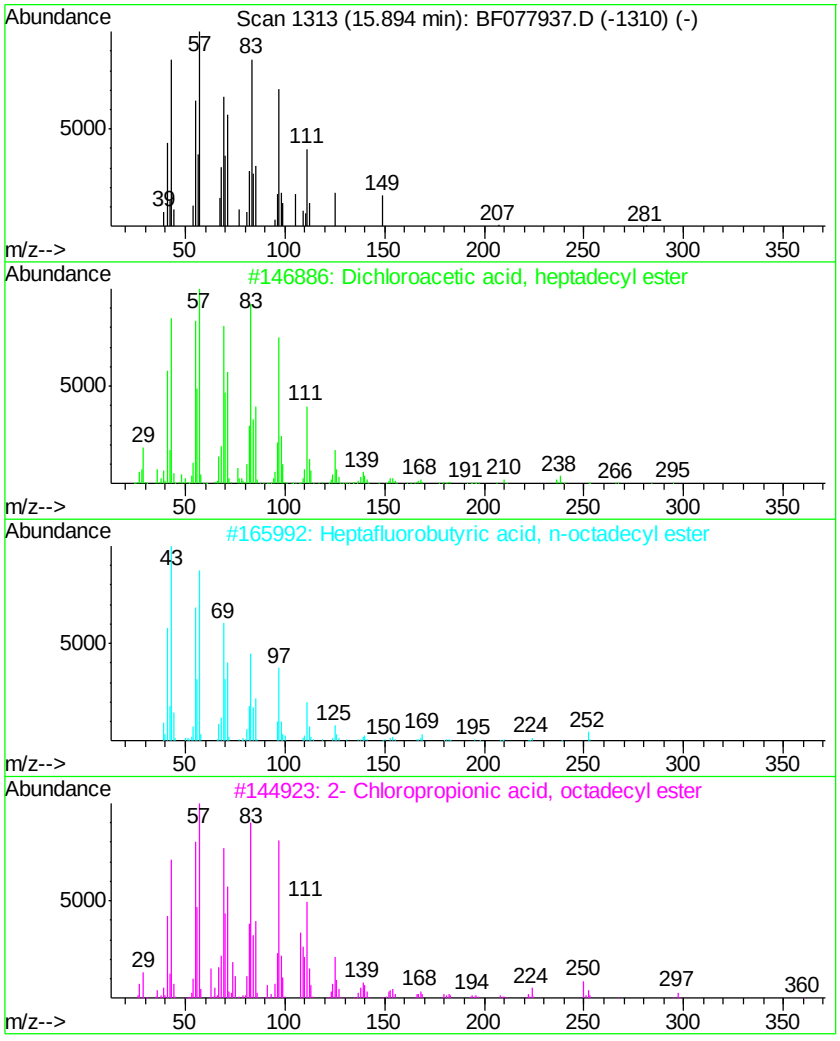
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

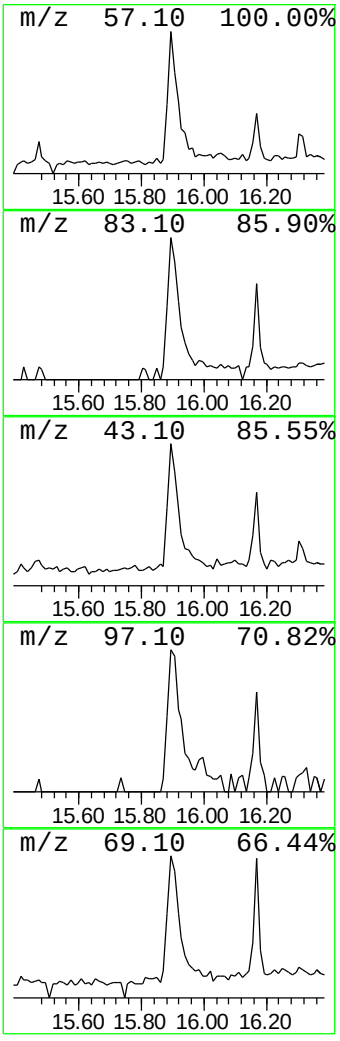
****

Peak Number 10 Dichloroacetic acid, heptad... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.89	4.40 ng	111204	Chrysene-d12	16.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	95
2	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91
3	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	91
4	Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	90
5	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	90





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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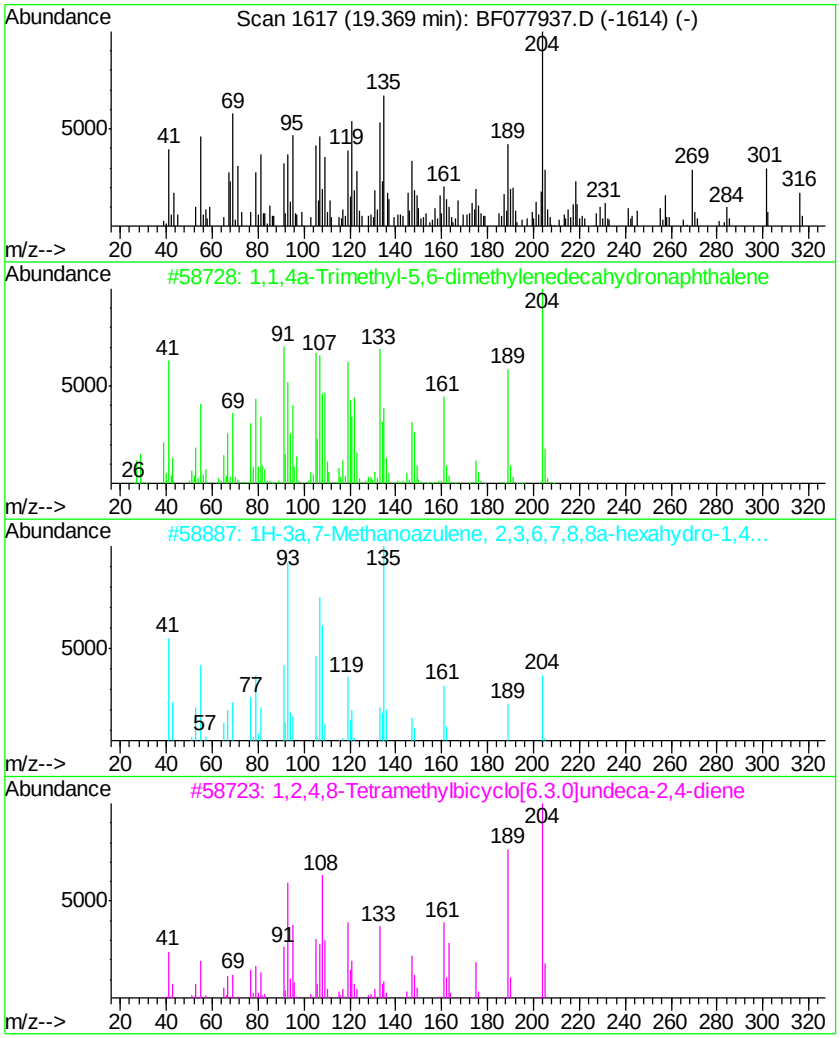
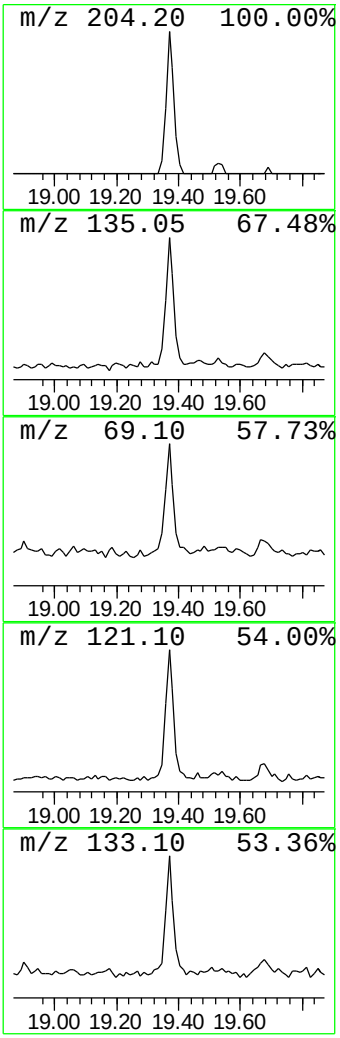
Peak Number 11 1,1,4a-Trimethyl-5,6-dimeth... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.37	11.83 ng	322386	Perylene-d12	17.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1,4a-Trimethyl-5,6-dimethylene...	204	C15H24	1000193-60-8	59
2	1H-3a,7-Methanoazulene, 2,3,6,7,...	204	C15H24	000560-32-7	53
3	1,2,4,8-Tetramethylbicyclo[6.3.0...	204	C15H24	137235-51-9	49
4	Farnesyl bromide	284	C15H25Br	006874-67-5	49
5	2,5,5,8a-Tetramethyl-6,7,8,8a-te...	204	C14H20O	124957-09-1	49





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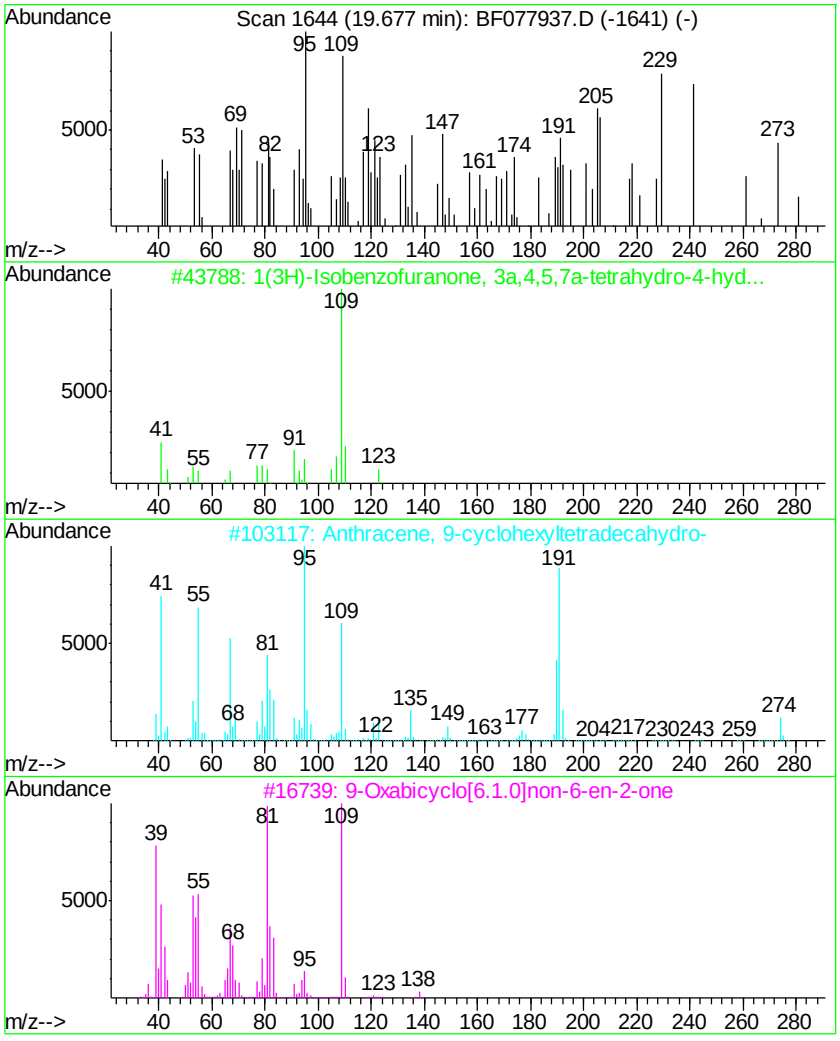
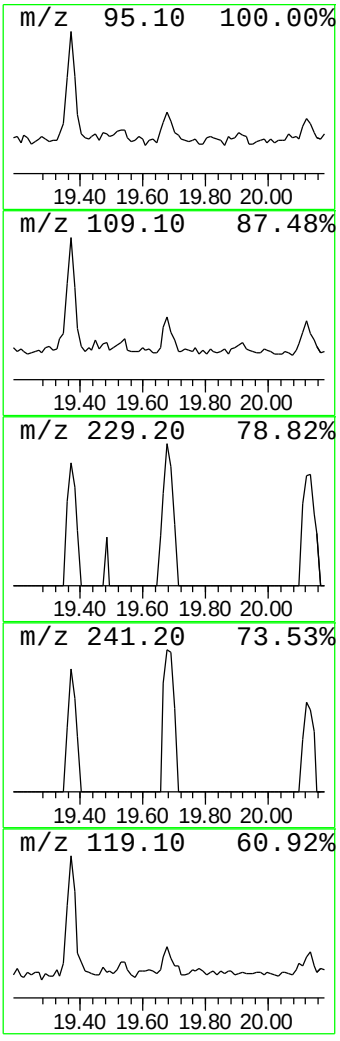
Peak Number 12 unknown19.68 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.68	2.24 ng	61042	Perylene-d12	17.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1(3H)-Isobenzofuranone, 3a,4,5,7...	182	C10H14O3	054346-06-4	27
2	Anthracene, 9-cyclohexyltetradec...	274	C20H34	055255-70-4	16
3	9-Oxabicyclo[6.1.0]non-6-en-2-one	138	C8H10O2	1000211-01-6	16
4	(1,3-Dimethyl-2-methylene-cyclop...	140	C9H16O	1000190-16-2	12
5	Pyridine, 3-methyl-, 1-oxide	109	C6H7NO	001003-73-2	12





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Instrument : BNA_F
ClientSampleId : SB-5-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031115.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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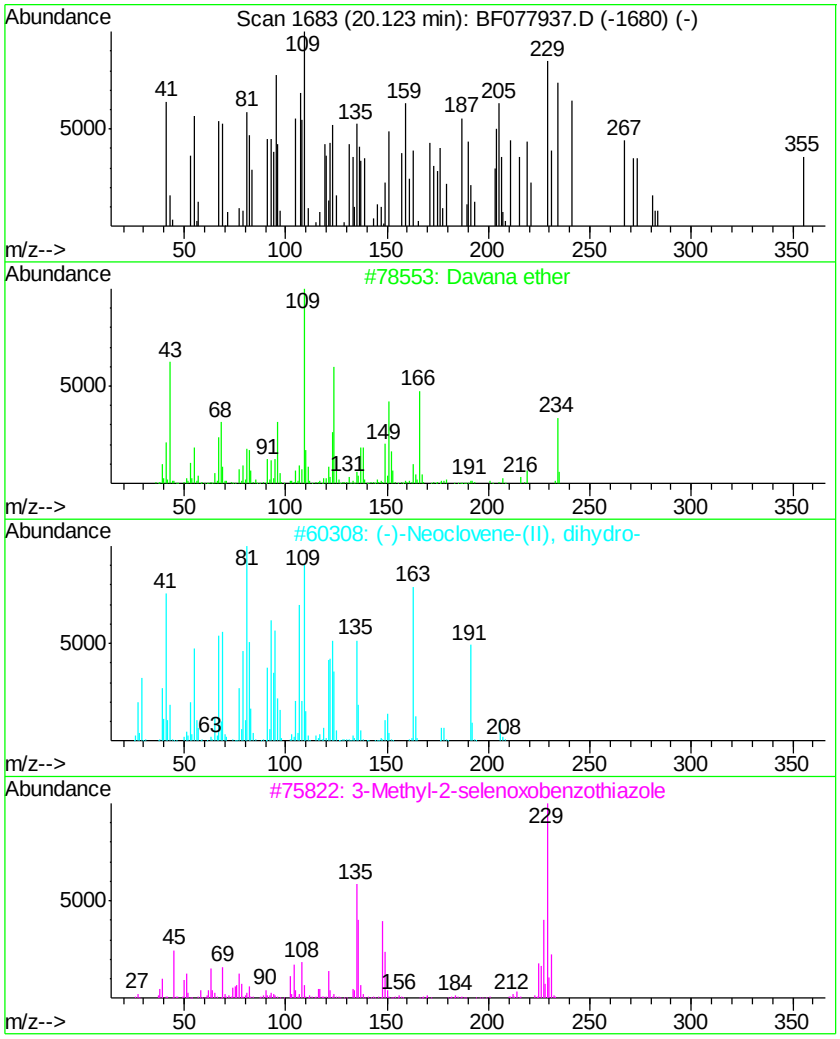
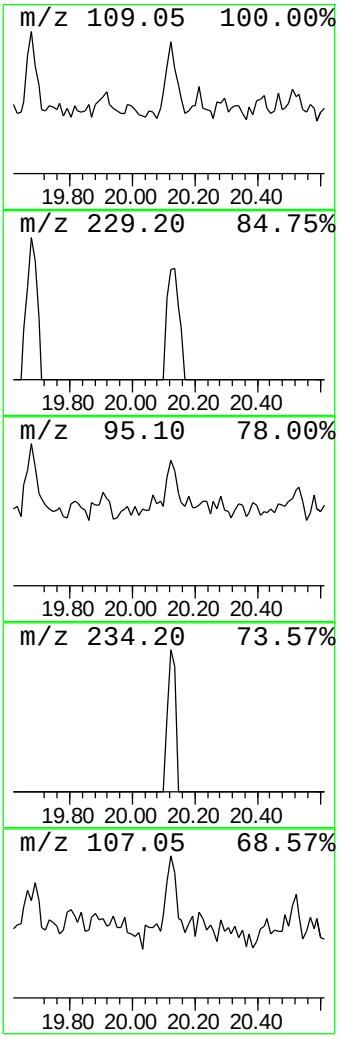
Peak Number 13 unknown20.12 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.12	2.31 ng	62929	Perylene-d12	17.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Davana ether	234	C15H22O2	035470-57-6	14
2	(-)-Neoclovene-(II), dihydro-	206	C15H26	1000152-83-6	14
3	3-Methyl-2-selenoxobenzothiazole	229	C8H7NSSe	002786-43-8	11
4	1H-1,2,4-Triazol-3-amine, 5-(2-t...	273	C10H10F3N5O	255872-85-6	11
5	Benzenamine, 2-ethyl-N-(4,4-dime...	234	C13H18N2S	1000272-26-2	11





Tentatively Identified Compound (LSC) summary

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Data File : BF077937.D
Acq On : 25 Mar 2015 5:32
Operator : TP/IZ
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Instrument : BNA_F
ClientSampleId : SB-5-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031115.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...	1.05	63.9	ng	824490	1	7.12	257992	20.0
Propane, 2,2-dime...	1.26	178.8	ng	2305880	1	7.12	257992	20.0
Butane, 2-methoxy...	1.55	6.8	ng	87256	1	7.12	257992	20.0
2-Pentanone, 4-hy...	4.86	8.4	ng	108322	1	7.12	257992	20.0
unknown6.83	6.83	75.8	ng	978208	1	7.12	257992	20.0
Dichloroacetic ac...	15.89	4.4	ng	111204	5	16.00	504991	20.0
1,1,4a-Trimethyl-...	19.37	11.8	ng	322386	6	17.80	544987	20.0
unknown19.68	19.68	2.2	ng	61042	6	17.80	544987	20.0
unknown20.12	20.12	2.3	ng	62929	6	17.80	544987	20.0