LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032415\
Data File : BF077931.D
Acq On : 25 Mar 2015 2:40
Operator : TP/IZ
Sample : G1613-01 5X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-1-1

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	12	14	27	rVB2	36925	102847	20.03%	2.077%
2	1.253	30	32	35	rVB	434782	414938	80.79%	8.379%
3	1.390	41	44	46	rVB	48169	74018	14.41%	1.495%
4	1.538	56	57	64	rVB	14548	22704	4.42%	0.458%
5	1.767	74	77	86	rVB	183860	297670	57.96%	6.011%
6	4.864	347	348	352	rBV2	10314	17529	3.41%	0.354%
7	5.402	393	395	404	rVB	113794	134166	26.12%	2.709%
8	6.693	505	508	518	rVB	120412	140609	27.38%	2.839%
9	6.830	518	520	522	rBV	156587	158875	30.93%	3.208%
10	7.116	543	545	547	rBV	240521	221632	43.15%	4.475%
11	7.299	559	561	564	rVB	148910	132593	25.82%	2.677%
12	7.813	603	606	608	rBV	66221	84602	16.47%	1.708%
13	8.693	681	683	685	rBV	319856	314707	61.28%	6.355%
14	10.042	799	801	803	rBV	188403	220040	42.84%	4.443%
15	10.865	870	873	875	rVB	295654	373572	72.74%	7.543%
16	11.448	919	924	926	rBV3	4848	10563	2.06%	0.213%
17	11.722	943	948	949	rBV4	3123	7877	1.53%	0.159%
18	11.836	956	958	965	rBV	104885	108086	21.05%	2.183%
19	12.042	974	976	981	rBV3	3675	6782	1.32%	0.137%
20	12.145	981	985	988	rBV4	4949	9542	1.86%	0.193%
21	12.694	1031	1033	1036	rBV	427892	419299	81.64%	8.467%
22	12.785	1039	1041	1043	rVB3	3376	6188	1.20%	0.125%
23	13.460	1098	1100	1103	rVB3	7165	8823	1.72%	0.178%
24	13.665	1110	1118	1121	rBV8	8187	35163	6.85%	0.710%
25	13.757	1125	1126	1130	rVB4	6624	7232	1.41%	0.146%
26	13.825	1130	1132	1133	rBV	6902	10272	2.00%	0.207%
27	14.180	1161	1163	1164	rBV2	5354	7935	1.55%	0.160%
28	14.214	1164	1166	1168	rVV	12326	16384	3.19%	0.331%
29	14.282	1169	1172	1175	rVB5	12669	18737	3.65%	0.378%
30	14.682	1205	1207	1210	rBV	236030	303436	59.08%	6.127%
31	15.974	1317	1320	1324	rBV	447423	513591	100.00%	10.371%
32	17.689	1468	1470	1474	rBV	340689	468535	91.23%	9.461%
33	18.226	1515	1517	1523	rVB4	49554	124336	24.21%	2.511%
34	19.232	1602	1605	1610	rVB4	89050	159017	30.96%	3.211%

LSC Area Percent Report

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Data File : BF077931.D
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Sample : G1613-01 5X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-1-1

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

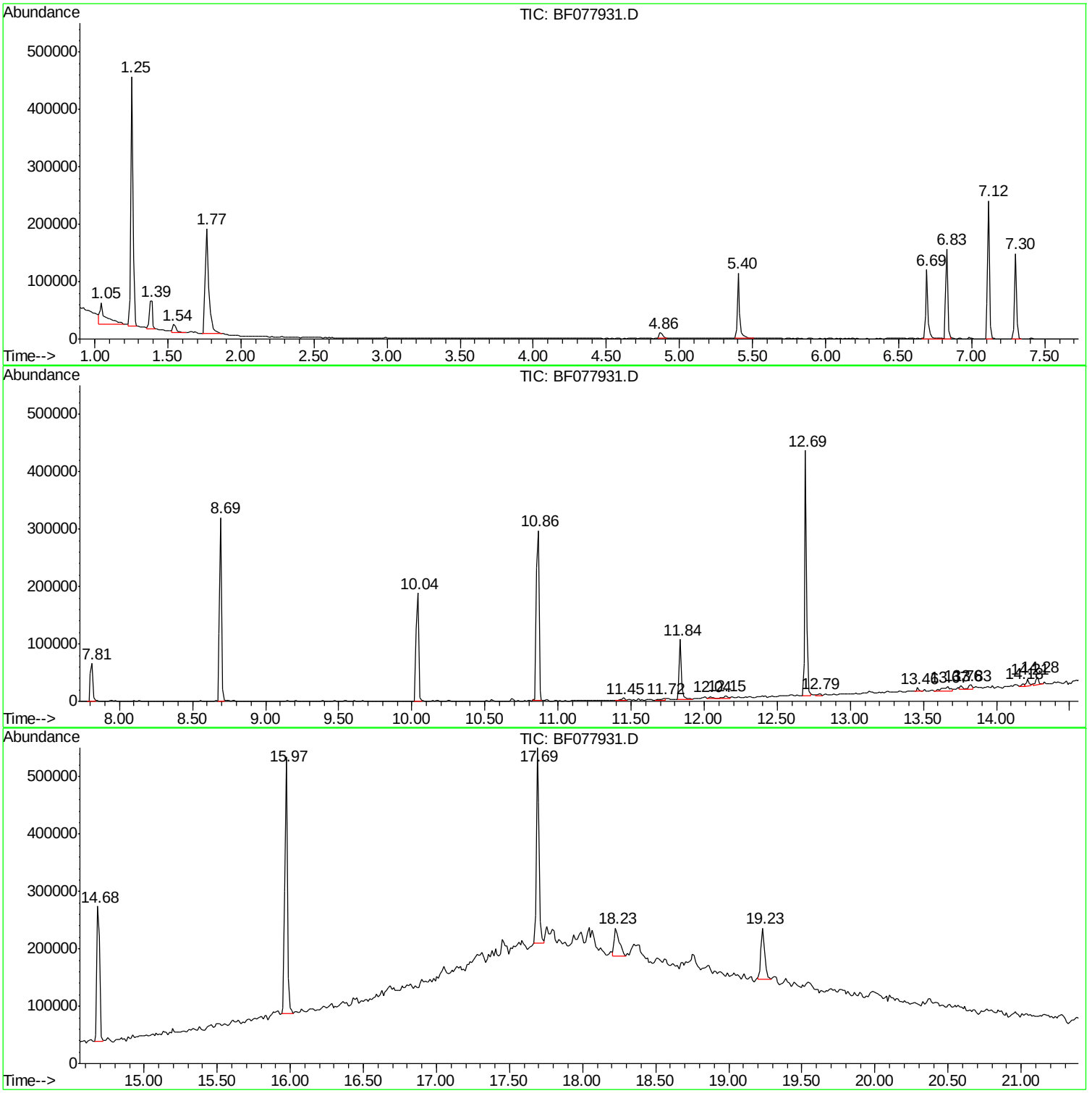
Sum of corrected areas: 4952300

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032415\
Data File : BF077931.D
Acq On : 25 Mar 2015 2:40
Operator : TP/IZ
Sample : G1613-01 5X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-1-1

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



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032415\
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Acq On : 25 Mar 2015 2:40
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

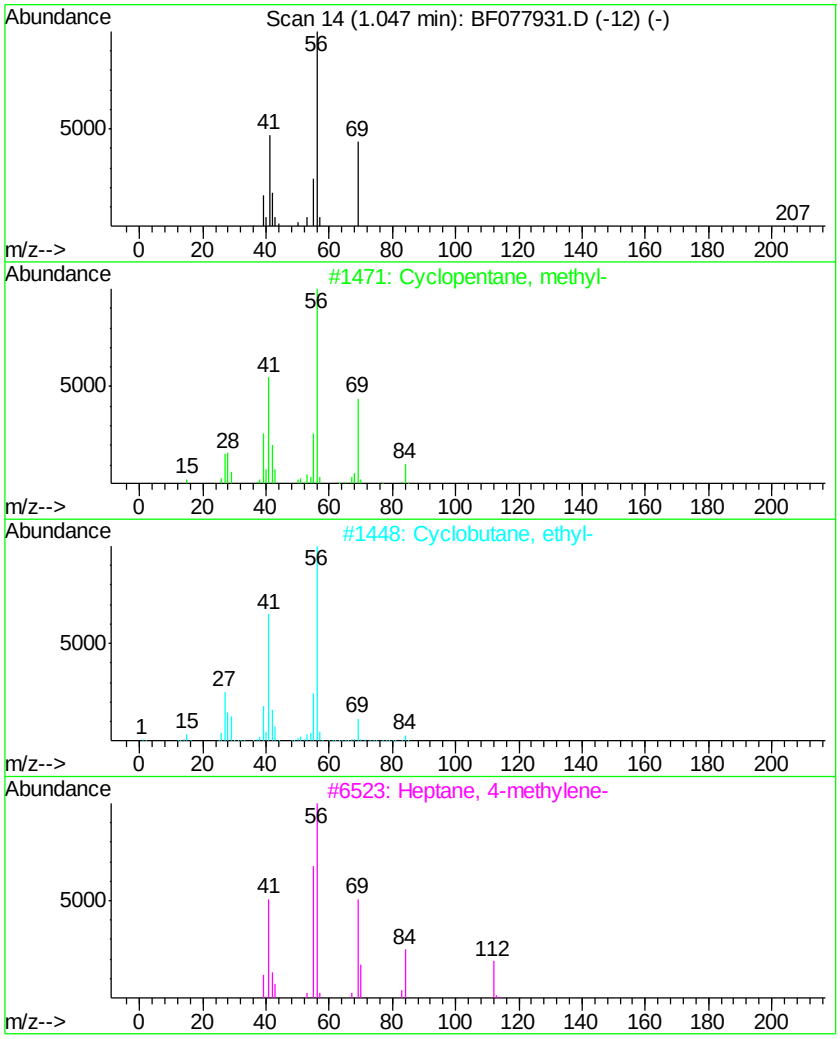
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

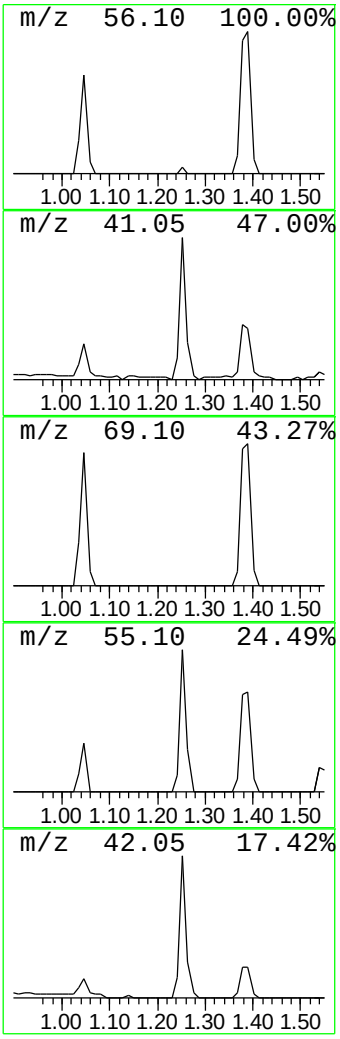
****

Peak Number 1 Cyclopentane, methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.05	9.28 ng	102847	1,4-Dichlorobenzene-d4	7.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	83
2	Cyclobutane, ethyl-	84	C6H12	004806-61-5	64
3	Heptane, 4-methylene-	112	C8H16	015918-08-8	40
4	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	40
5	cis-4,6-Dimethylcyclohexane-1,3-...	140	C8H12O2	069841-15-2	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032415\
Data File : BF077931.D
Acq On : 25 Mar 2015 2:40
Operator : TP/IZ
Sample : G1613-01 5X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-1-1

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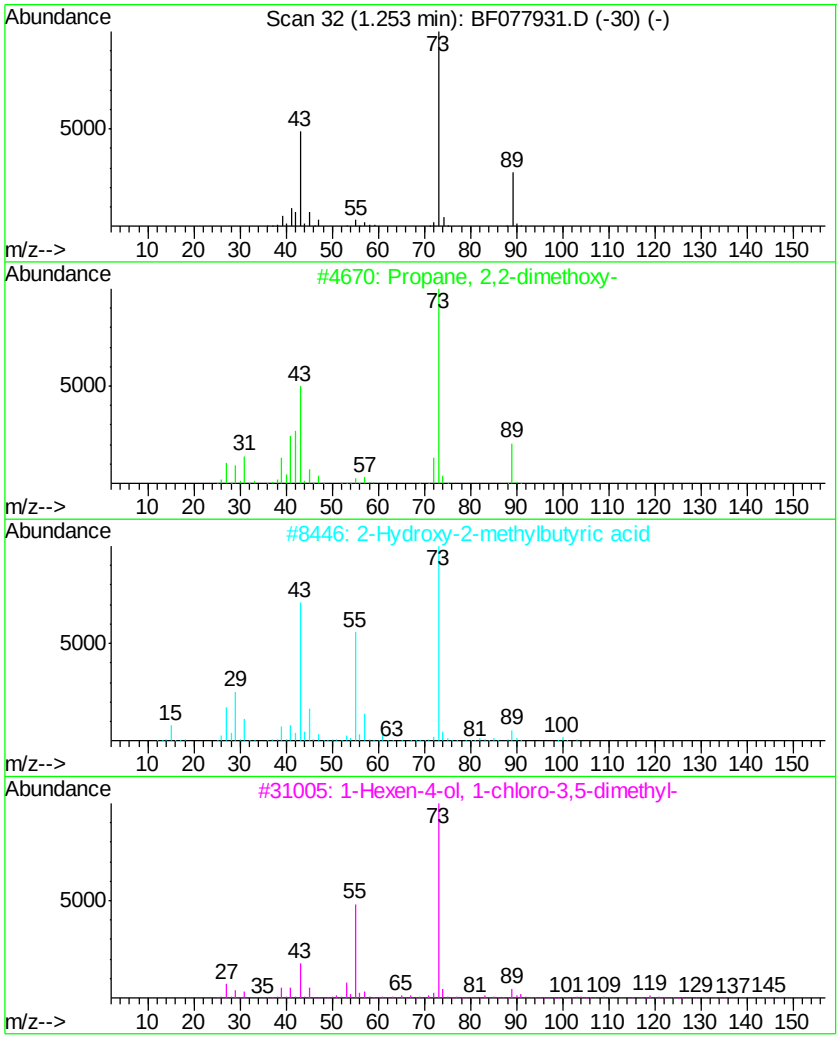
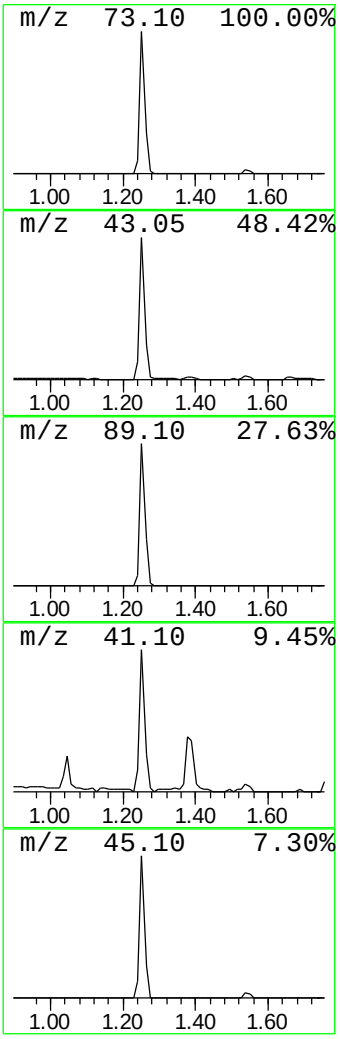
Peak Number 2 Propane, 2,2-dimethoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.25	37.44 ng	414938	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	50
2	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9
3	1-Hexen-4-ol, 1-chloro-3,5-dimet...	162	C8H15ClO	100244-09-5	9
4	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
5	Methane, isothiocyanato-	73	C2H3NS	000556-61-6	7





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Data File : BF077931.D
Acq On : 25 Mar 2015 2:40
Operator : TP/IZ
Sample : G1613-01 5X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-1-1

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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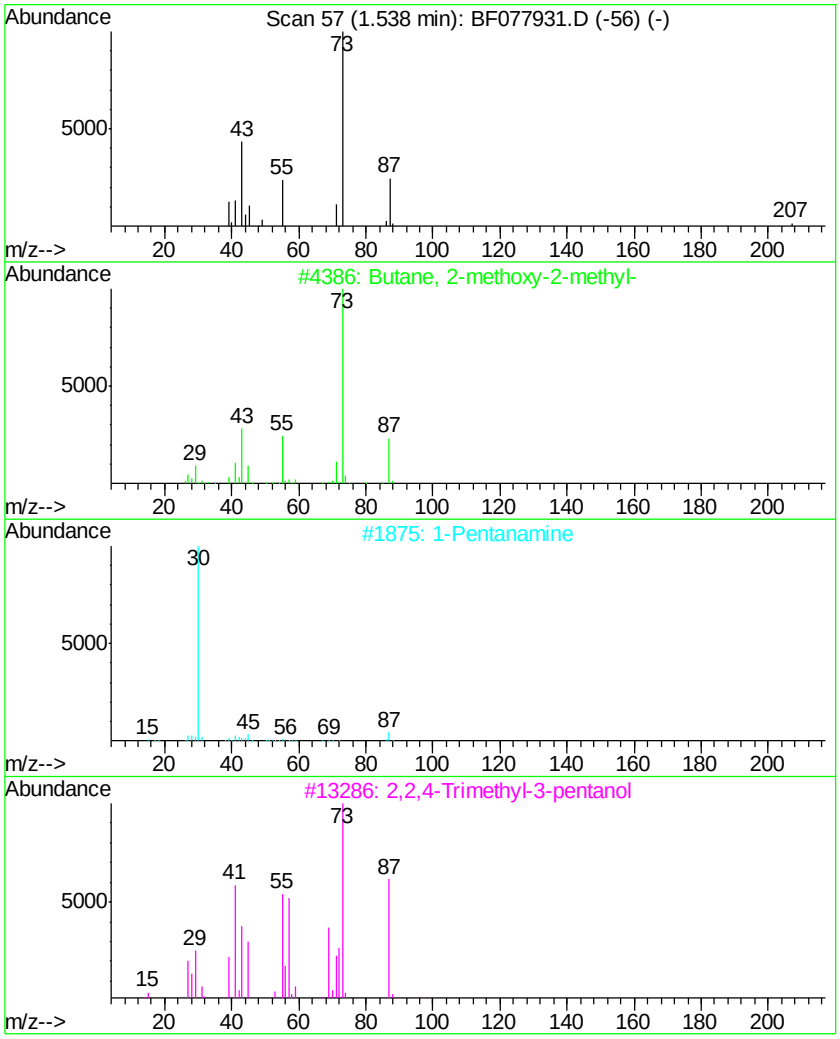
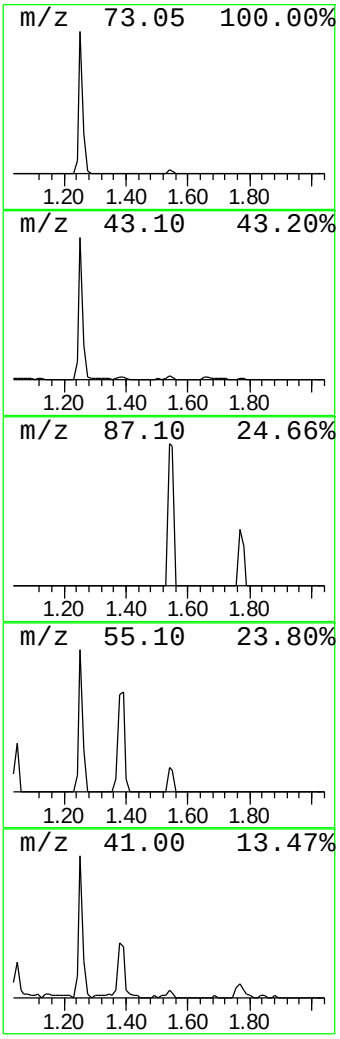
Peak Number 4 Butane, 2-methoxy-2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.54	2.05 ng	22704	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	64
2	1-Pentanamine	87	C5H13N	000110-58-7	9
3	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	9
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	7
5	Isobutylamine	73	C4H11N	000078-81-9	5





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032415\
Data File : BF077931.D
Acq On : 25 Mar 2015 2:40
Operator : TP/IZ
Sample : G1613-01 5X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-1-1

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

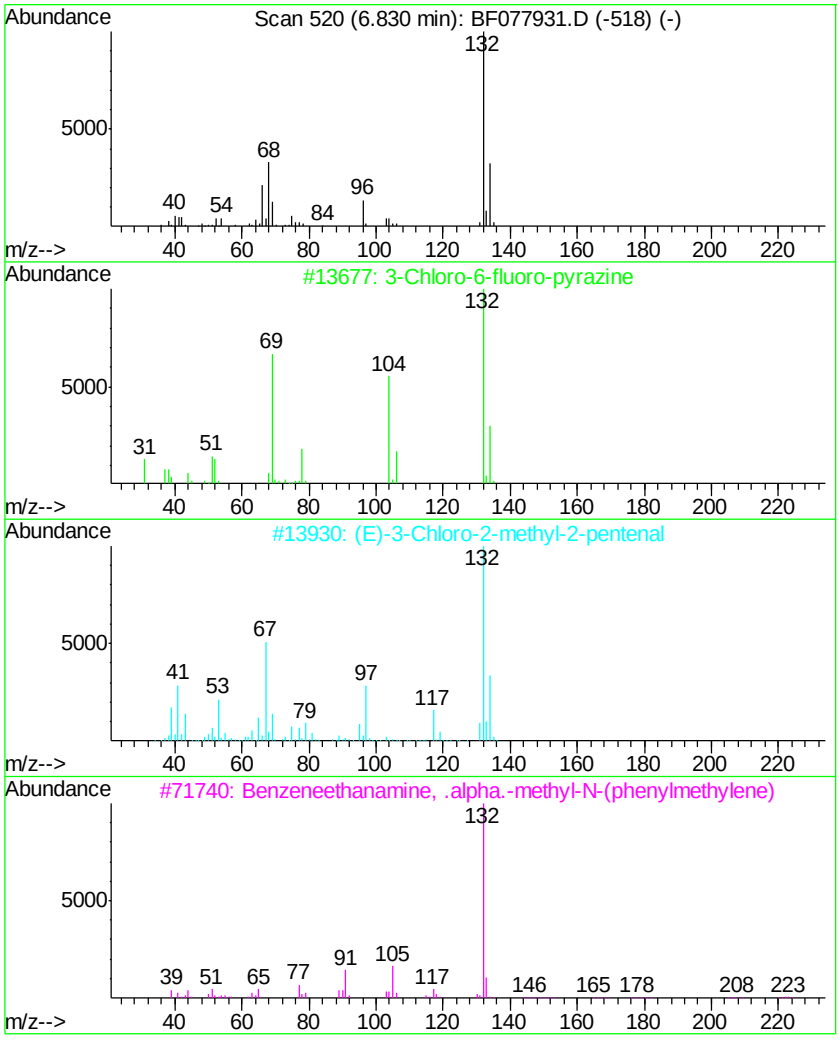
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

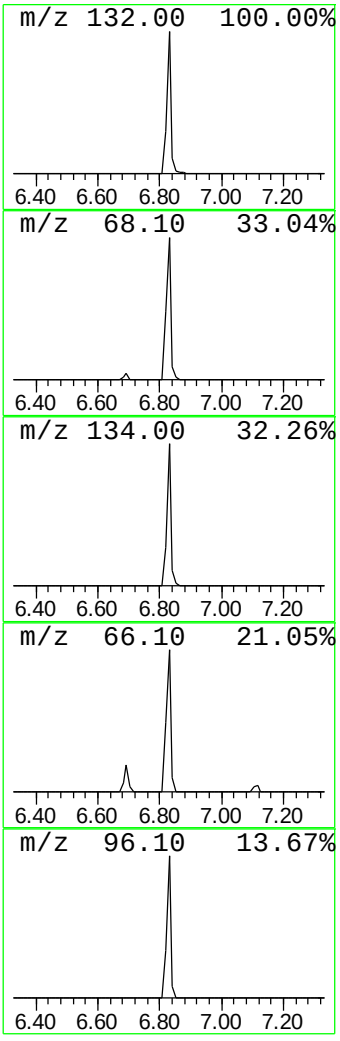
****

Peak Number 6 unknown6.83 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.83	14.34 ng	158875	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	38
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
3	Benzeneethanamine, .alpha.-methy...	223	C16H17N	002980-02-1	12
4	Amphetaminil	250	C17H18N2	017590-01-1	12
5	5-Aminoindole	132	C8H8N2	005192-03-0	10





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Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-1-1

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

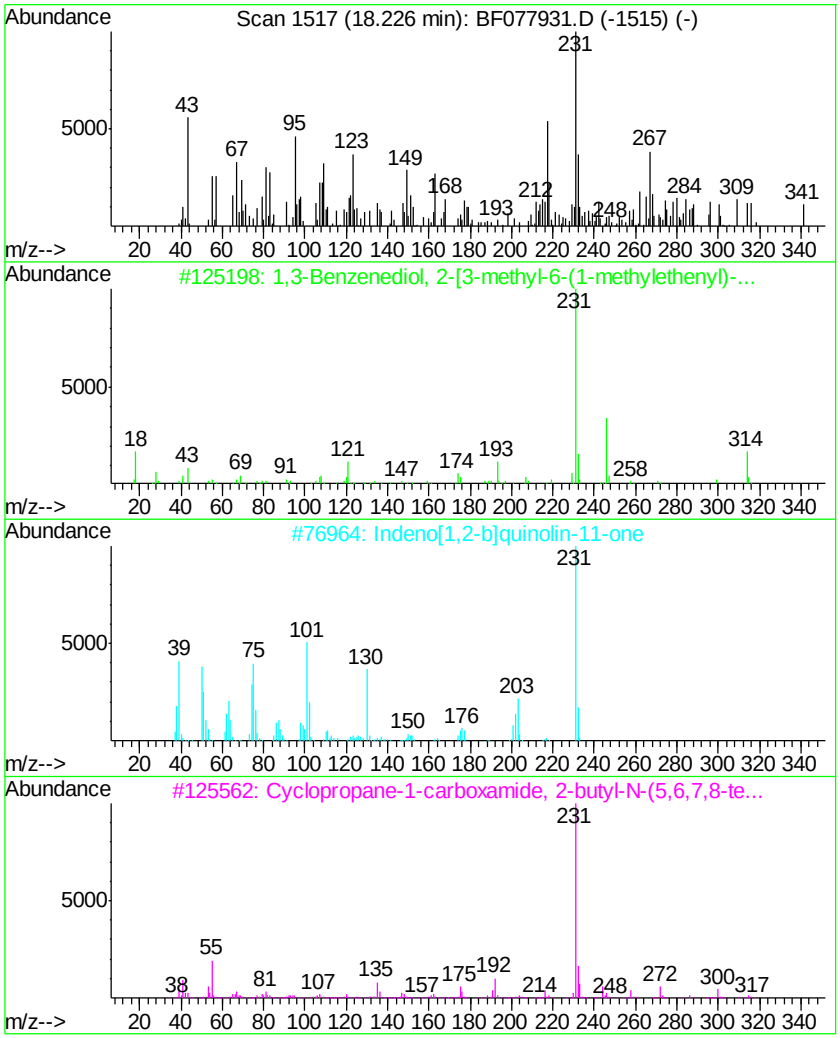
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

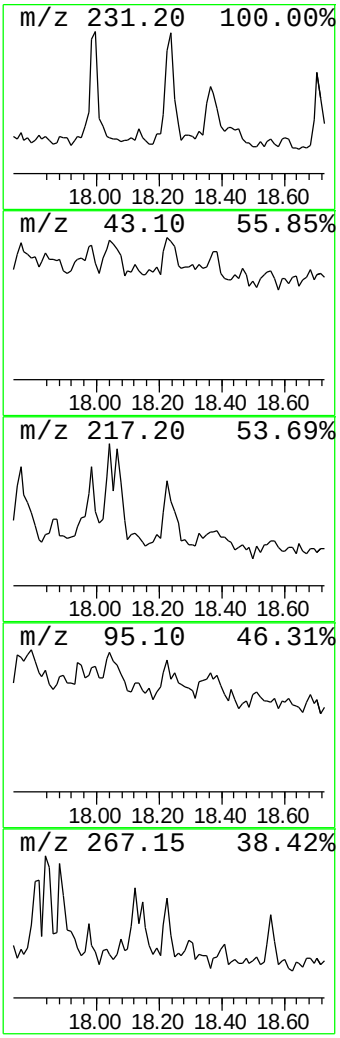
****

Peak Number 8 unknown18.23 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.23	5.31 ng	124336	Perylene-d12	17.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Benzenediol, 2-[3-methyl-6-(...	314	C21H30O2	013956-29-1	25
2	Indeno[1,2-b]quinolin-11-one	231	C16H9NO	100004-82-8	22
3	Cyclopropane-1-carboxamide, 2-bu...	315	C18H25N3O2	340695-72-9	22
4	2-[1-(2-[1,3]Dithian-2-yl-ethyl)...	316	C16H28O2S2	1000194-86-3	22
5	2,3(1H)-Dihydro-7-methylthio-9-c...	231	C13H13NOS	1000257-08-5	18





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Misc :
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Instrument : BNA_F
ClientSampleId : SB-1-1

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

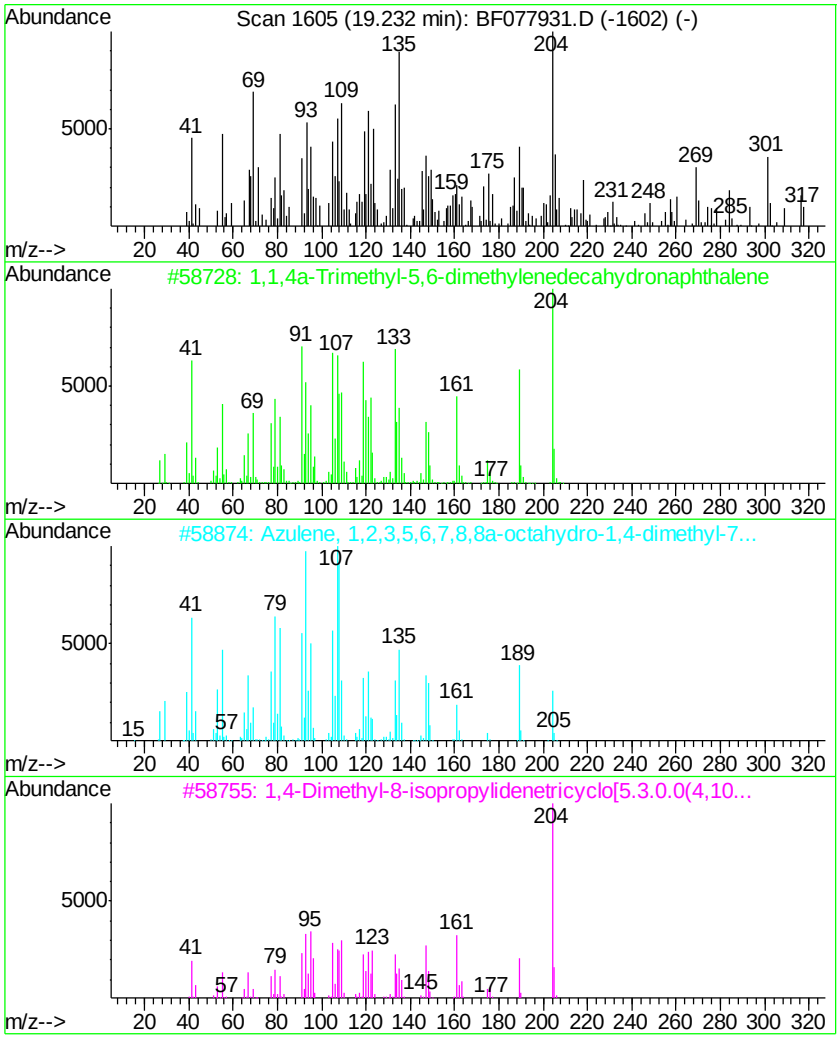
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

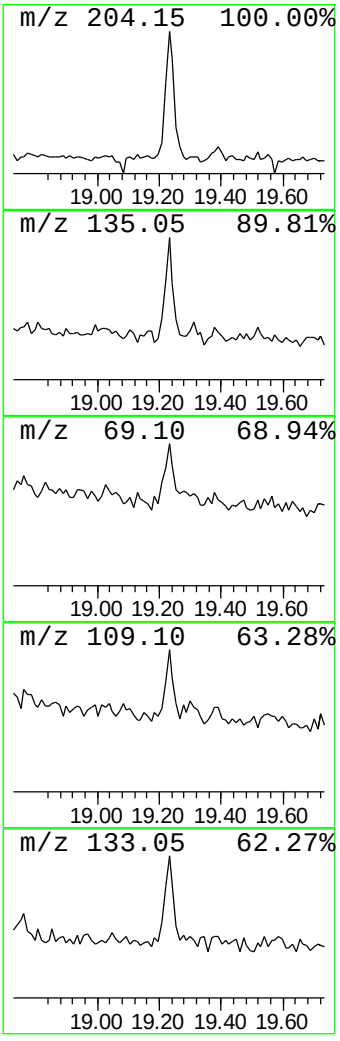
****

Peak Number 9 1,1,4a-Trimethyl-5,6-dimeth... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.23	6.79 ng	159017	Perylene-d12	17.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1,4a-Trimethyl-5,6-dimethylene...	204	C15H24	1000193-60-8	62
2	Azulene, 1,2,3,5,6,7,8,8a-octahy...	204	C15H24	003691-11-0	58
3	1,4-Dimethyl-8-isopropylidenetri...	204	C15H24	1000140-07-7	58
4	Naphthalene, decahydro-4a-methyl...	204	C15H24	017066-67-0	55
5	Guaia-3,9-diene	204	C15H24	000489-83-8	49





Tentatively Identified Compound (LSC) summary

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Instrument : BNA_F
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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	9.3	ng	102847	1	7.12	221632	20.0
Propane, 2,2-dime...	1.25	37.4	ng	414938	1	7.12	221632	20.0
Butane, 2-methoxy...	1.54	2.0	ng	22704	1	7.12	221632	20.0
unknown6.83	6.83	14.3	ng	158875	1	7.12	221632	20.0
unknown18.23	18.23	5.3	ng	124336	6	17.69	468535	20.0
1,1,4a-Trimethyl-...	19.23	6.8	ng	159017	6	17.69	468535	20.0