LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF060516\
Data File : BF087722.D
Acq On : 5 Jun 2016 22:22
Operator : UM/SJ
Sample : H3379-13
Misc :
ALS Vial : 61 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-4

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-BF060416.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	1.758	11	15	17	rBV	4057969	7846661	100.00%	19.493%
2	1.907	26	28	48	rVB	1925262	3748380	47.77%	9.312%
3	2.147	48	49	77	rVB2	95918	334267	4.26%	0.830%
4	3.210	140	142	155	rBV	43265	100340	1.28%	0.249%
5	5.050	301	303	309	rVB	190517	300144	3.83%	0.746%
6	5.461	336	339	341	rBV	2635829	2900453	36.96%	7.206%
7	6.490	425	429	431	rBV	2439002	2844003	36.24%	7.065%
8	6.627	438	441	443	rBV	2852505	3025966	38.56%	7.517%
9	6.856	459	461	464	rBV	797924	682774	8.70%	1.696%
10	7.016	472	475	477	rVB	2581770	2397031	30.55%	5.955%
11	7.427	507	511	513	rBV	1675058	2199871	28.04%	5.465%
12	8.147	571	574	576	rBV	787670	934233	11.91%	2.321%
13	9.222	665	668	671	rBV	2890818	3218784	41.02%	7.996%
14	9.622	700	703	705	rBV	505787	611319	7.79%	1.519%
15	9.896	725	727	730	rVB	1141991	1034434	13.18%	2.570%
16	10.685	793	796	799	rBV	2007387	2051391	26.14%	5.096%
17	11.382	854	857	859	rBV	1051831	1041429	13.27%	2.587%
18	12.799	978	981	983	rBV	192107	205412	2.62%	0.510%
19	12.971	993	996	998	rBV	2866752	3052082	38.90%	7.582%
20	13.496	1040	1042	1045	rBV	127508	131033	1.67%	0.326%
21	13.874	1073	1075	1085	rBV	50794	107114	1.37%	0.266%
22	14.011	1085	1087	1089	rBV	931404	851534	10.85%	2.115%
23	15.440	1209	1212	1215	rBV	530950	634376	8.08%	1.576%

Sum of corrected areas: 40253031

LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF060516\
Data File : BF087722.D
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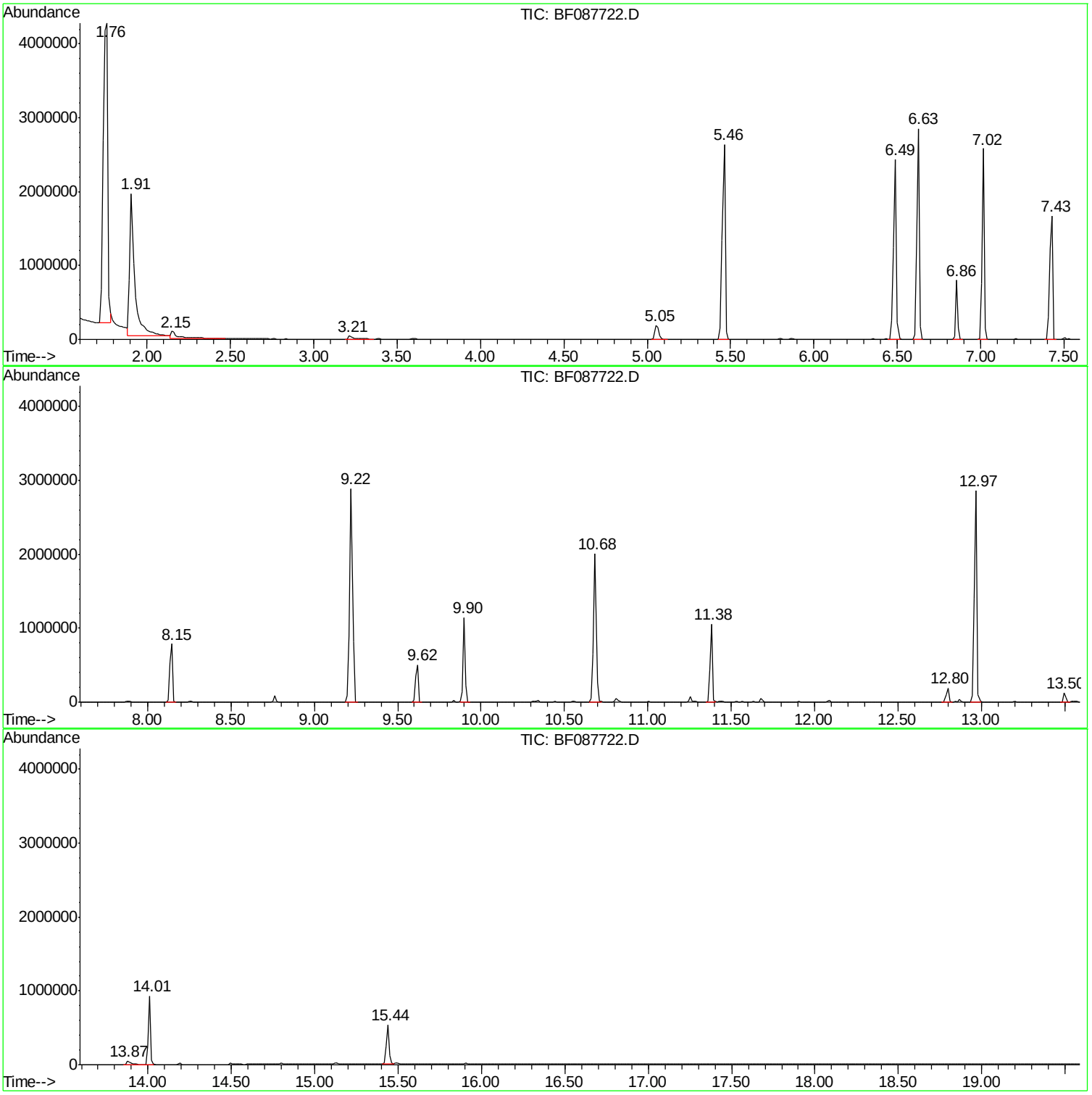
Operator : UM/SJ
Sample : H3379-13
Misc :
ALS Vial : 61 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\HPCHEM1\BNA F\DATA\BF060516\
Data File : BF087722.D
Acq On : 5 Jun 2016 22:22
Operator : UM/SJ
Sample : H3379-13
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

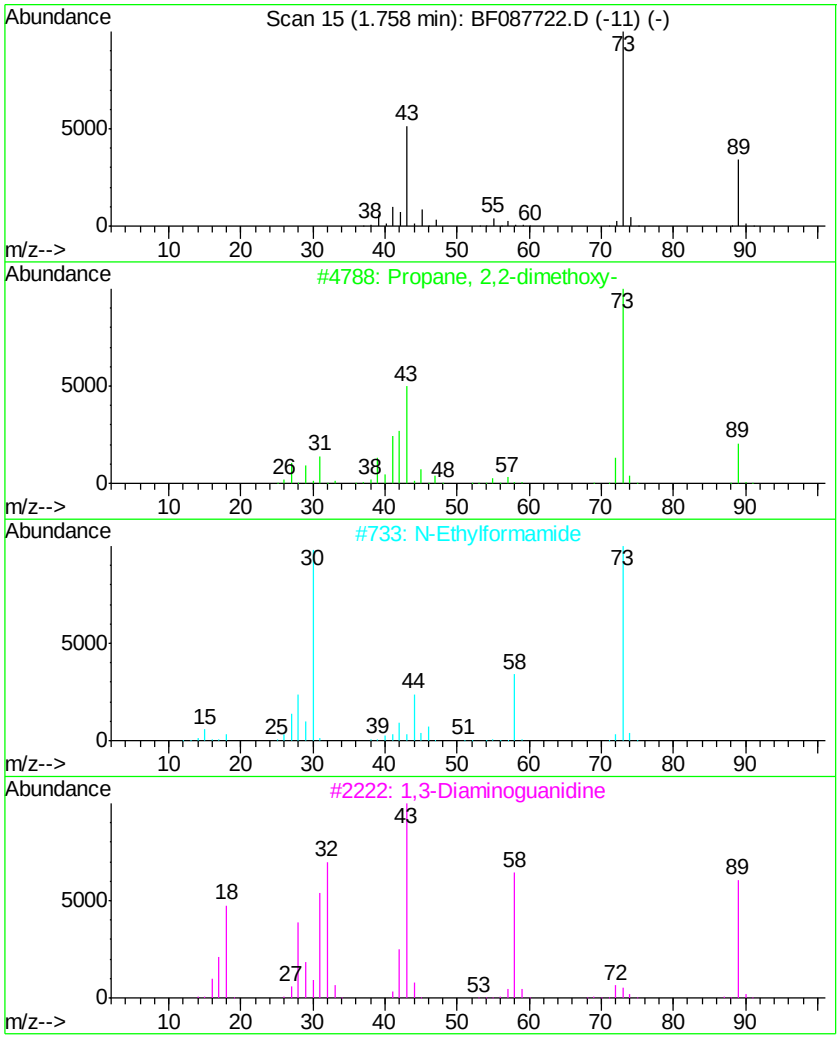
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

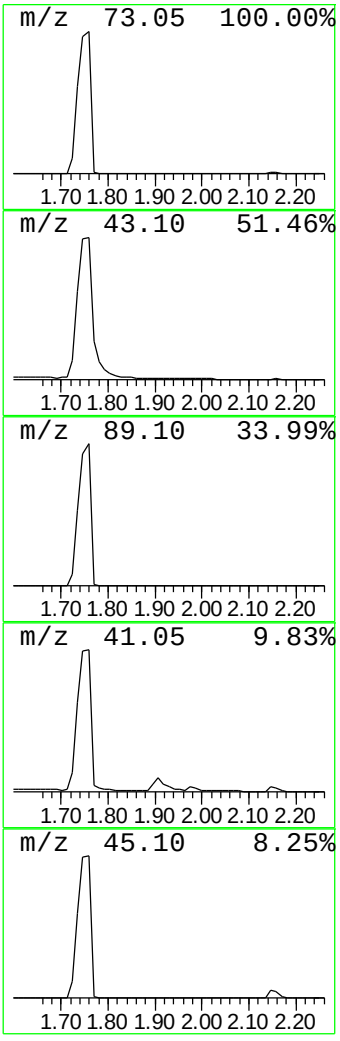
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.76	229.85 ng	7846660	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	56
2	N-Ethylformamide	73	C3H7NO	000627-45-2	9
3	1,3-Diaminoguanidine	89	CH7N5	004364-78-7	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 : BF087722.D
Acq On : 5 Jun 2016 22:22
Operator : UM/SJ
Sample : H3379-13
Misc :
ALS Vial : 61 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

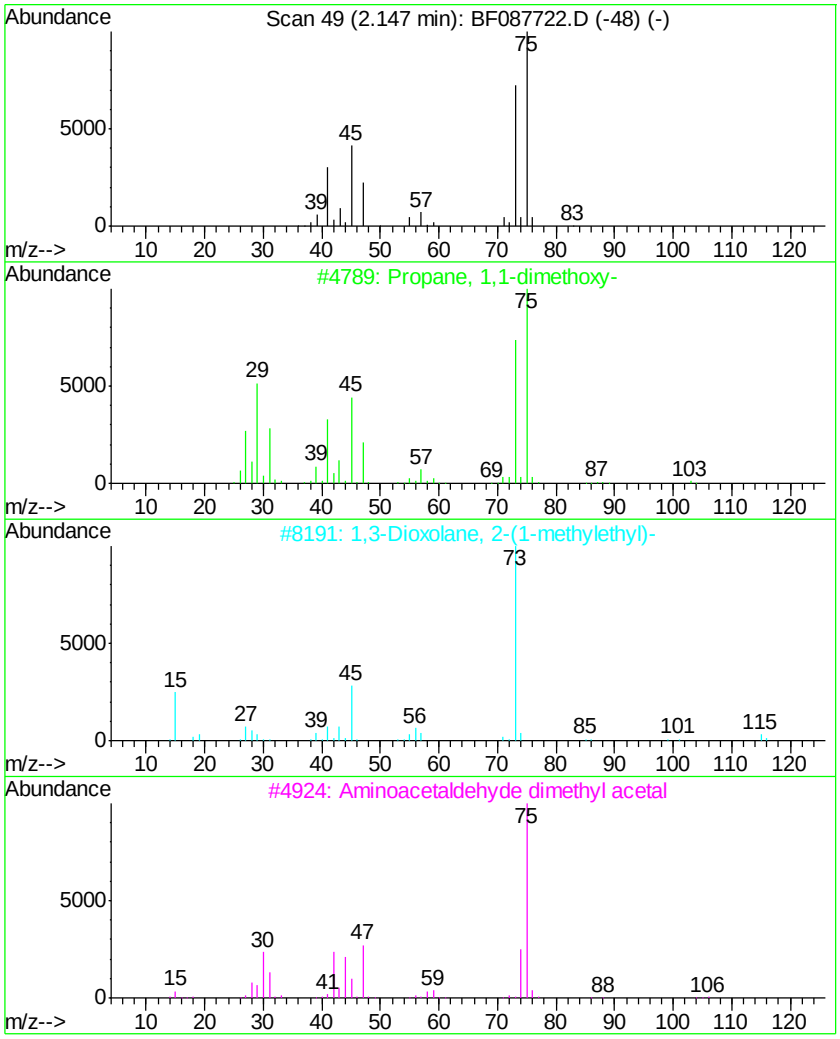
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

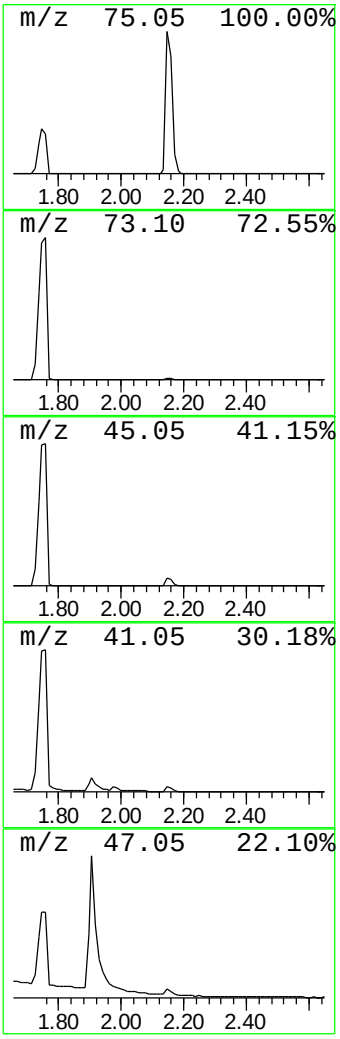
****

Peak Number 3 Propane, 1,1-dimethoxy- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.15	9.79 ng	334267	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	64
2	1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	12
3	Aminoacetaldehyde dimethyl acetal	105	C4H11NO2	022483-09-6	9
4	1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	9
5	Glycolaldehyde dimethyl acetal	106	C4H10O3	030934-97-5	9





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Acq On : 5 Jun 2016 22:22
Operator : UM/SJ
Sample : H3379-13
Misc :
ALS Vial : 61 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

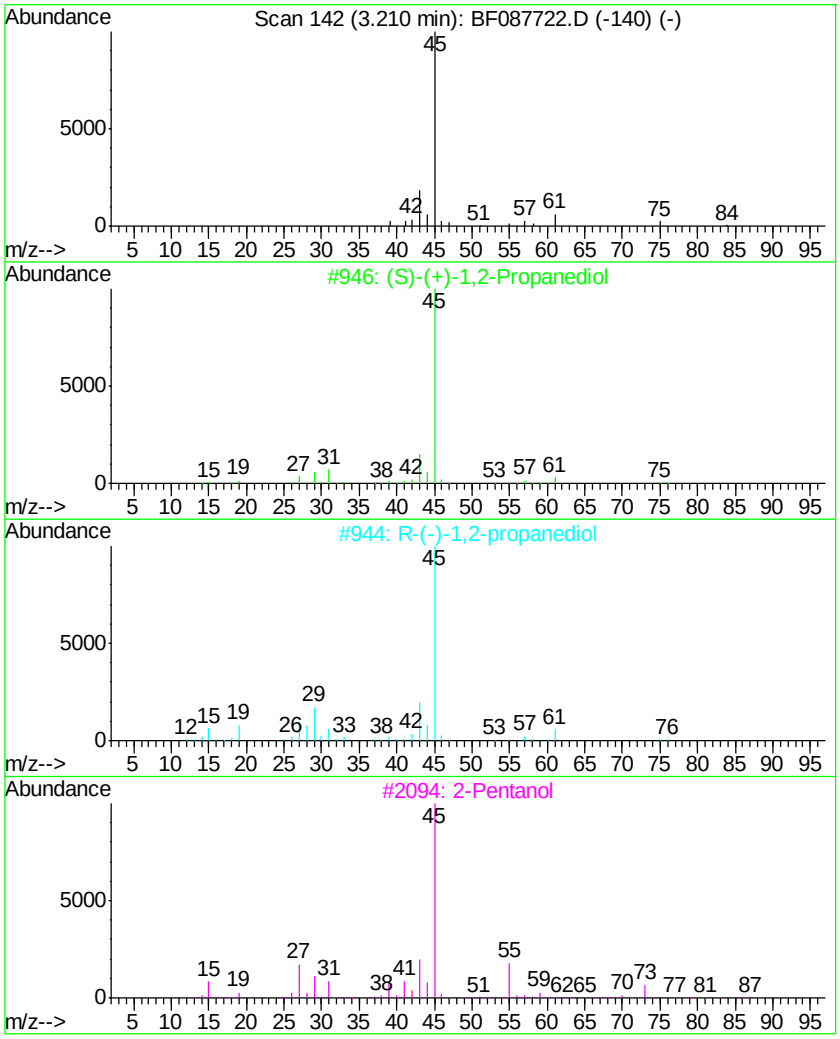
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

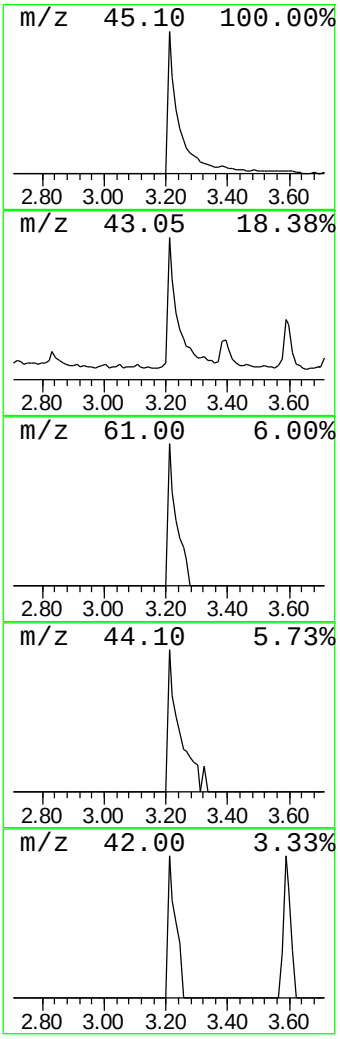
****

Peak Number 4 (S)-(+)-1,2-Propanediol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.21	2.94 ng	100340	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	56
2	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	40
3	2-Pentanol	88	C5H12O	006032-29-7	9
4	Propylene Glycol	76	C3H8O2	000057-55-6	9
5	Muramic acid	251	C9H17NO7	001114-41-6	9





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Instrument : BNA_F
ClientSampleId : SB-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

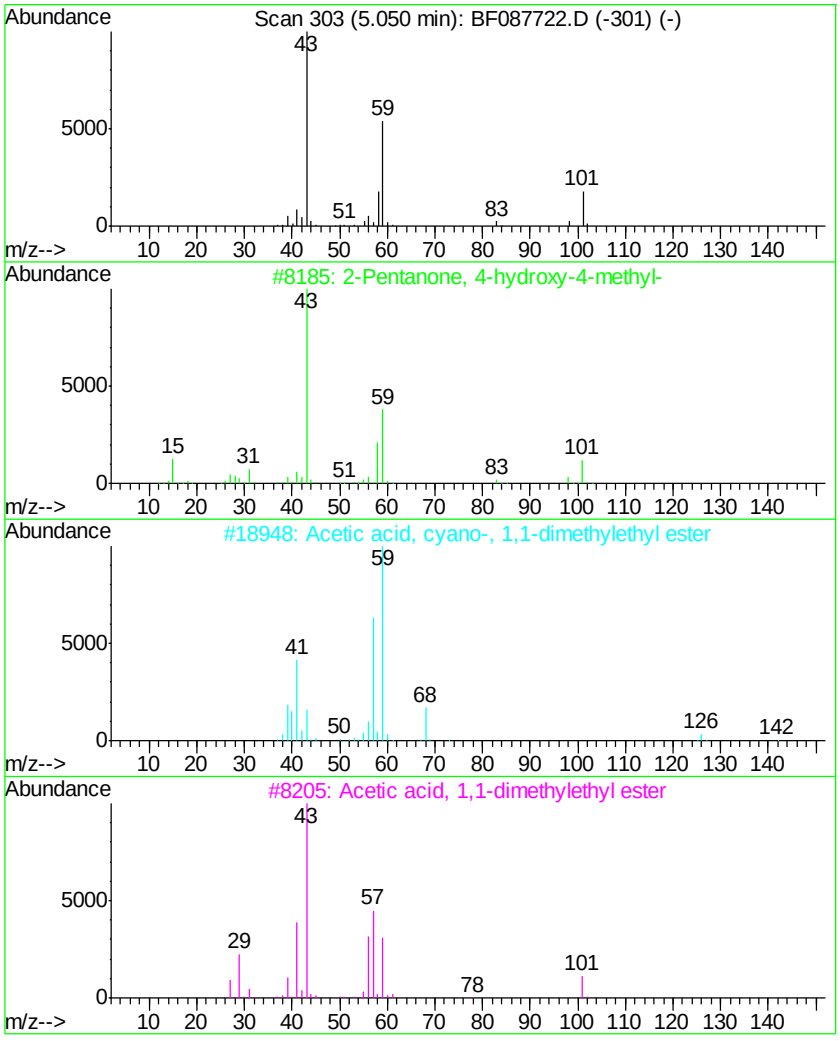
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

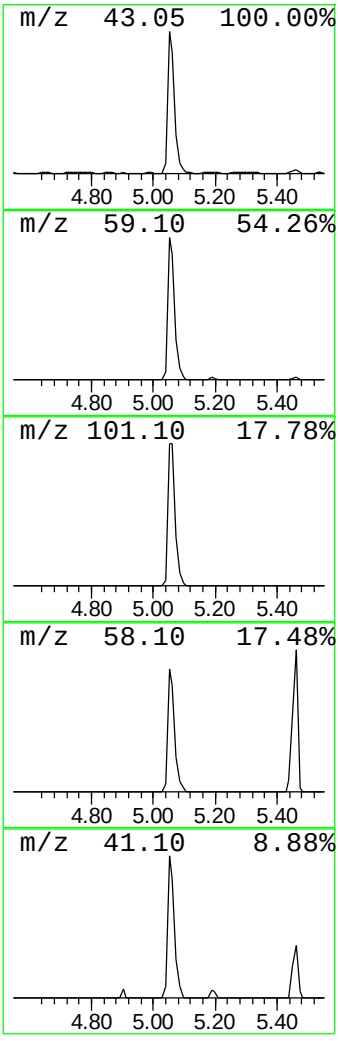
****

Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.05	8.79 ng	300144	1,4-Dichlorobenzene-d4	6.86

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	37
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10





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Operator : UM/SJ
Sample : H3379-13
Misc :
ALS Vial : 61 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

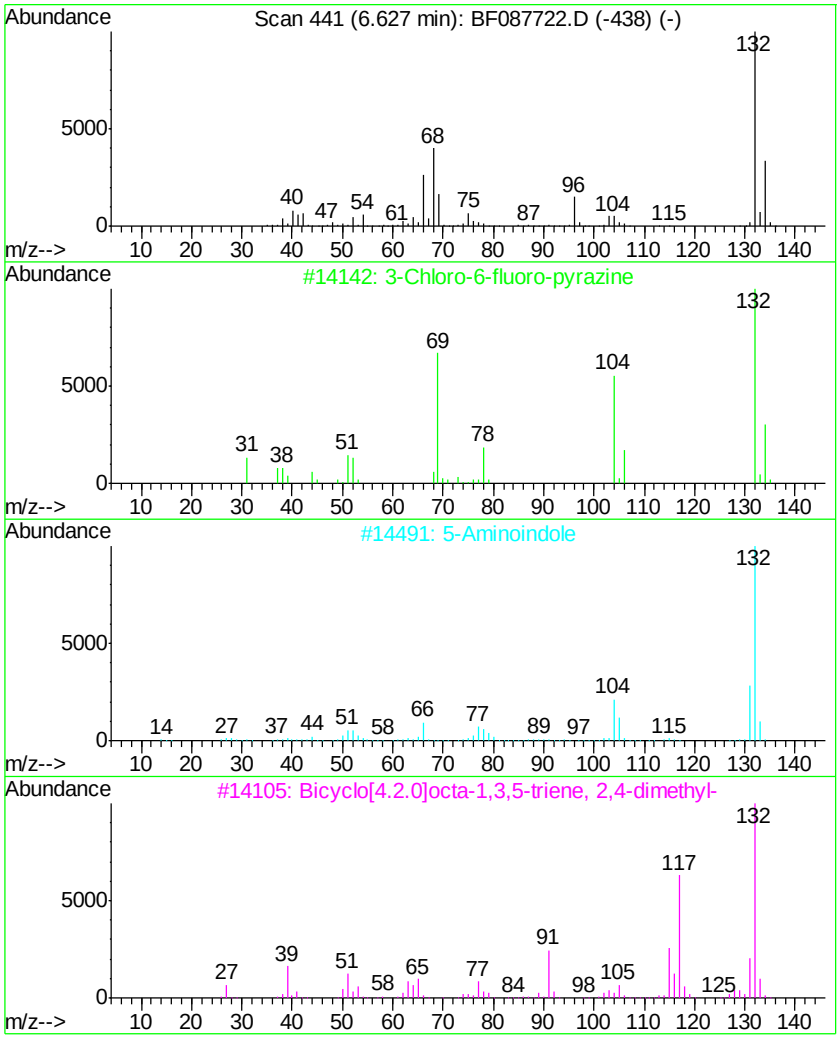
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

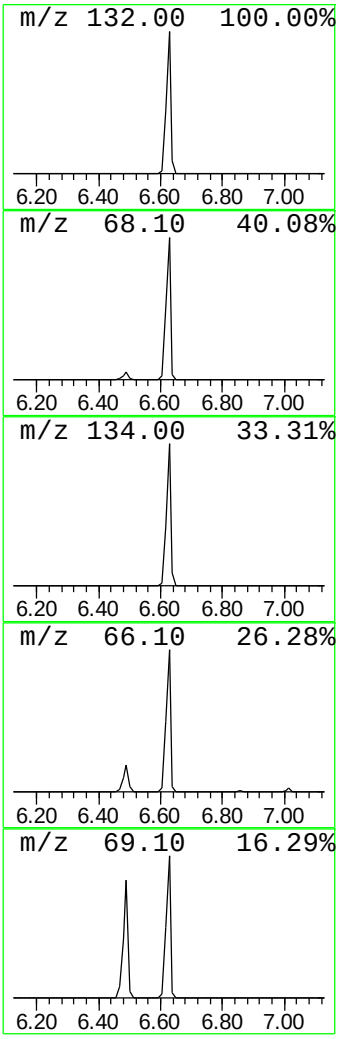
****

Peak Number 6 unknown6.63 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	88.64 ng	3025970	1,4-Dichlorobenzene-d4	6.86

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	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





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Operator : UM/SJ
Sample : H3379-13
Misc :
ALS Vial : 61 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

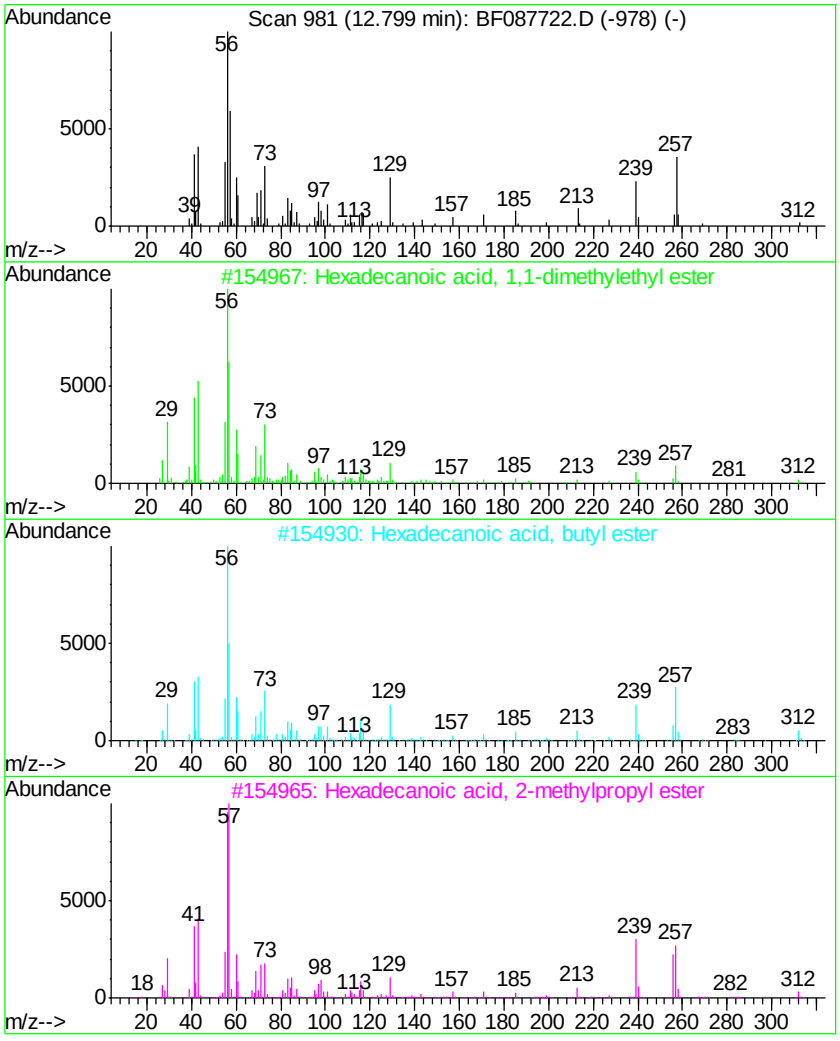
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

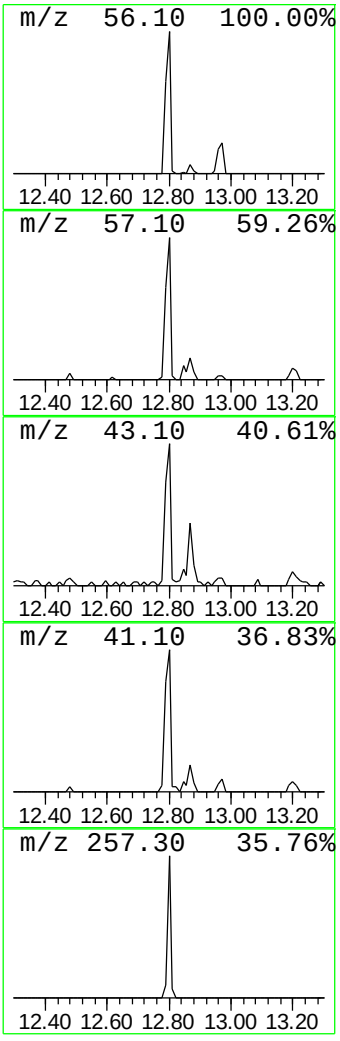
****

Peak Number 8 Hexadecanoic acid, 1,1-dime... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.80	4.82 ng	205412	Chrysene-d12	14.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	96
2	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
3	Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	43
4	Butyl 4,8,12-trimethyl-tridecanoate	312	C20H40O2	1000336-63-2	27
5	Cyclohexanol, 4-amino-, trans-	115	C6H13NO	027489-62-9	25





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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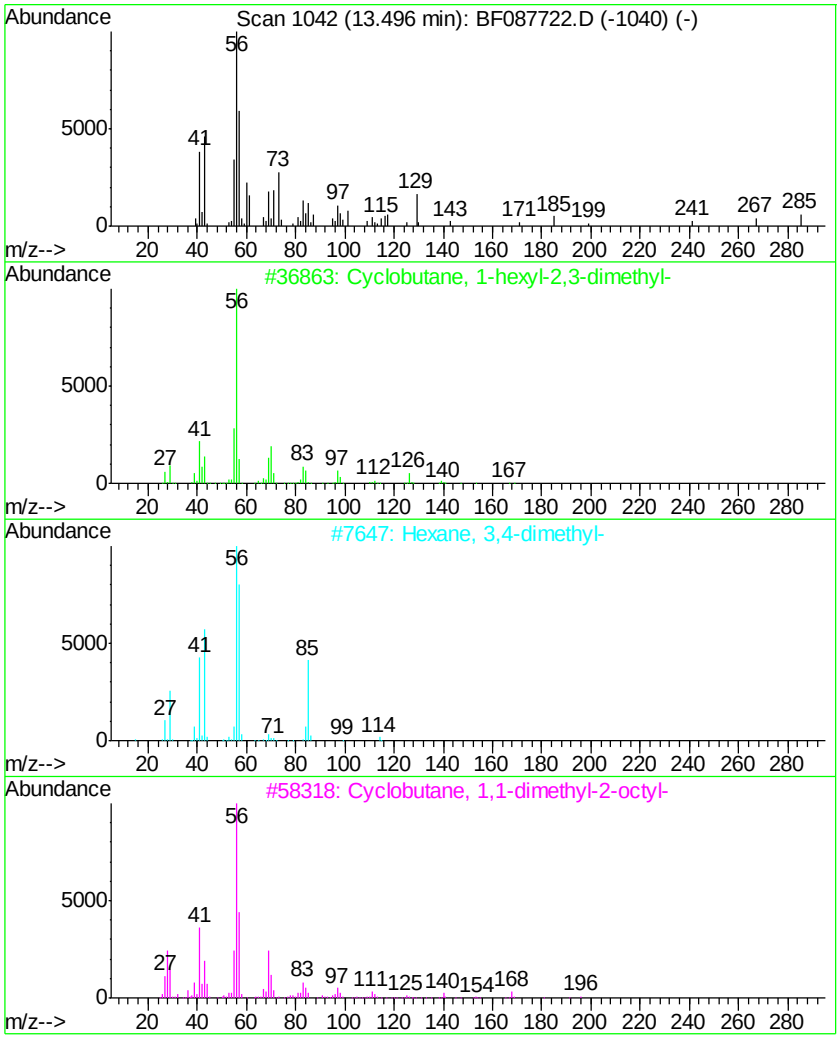
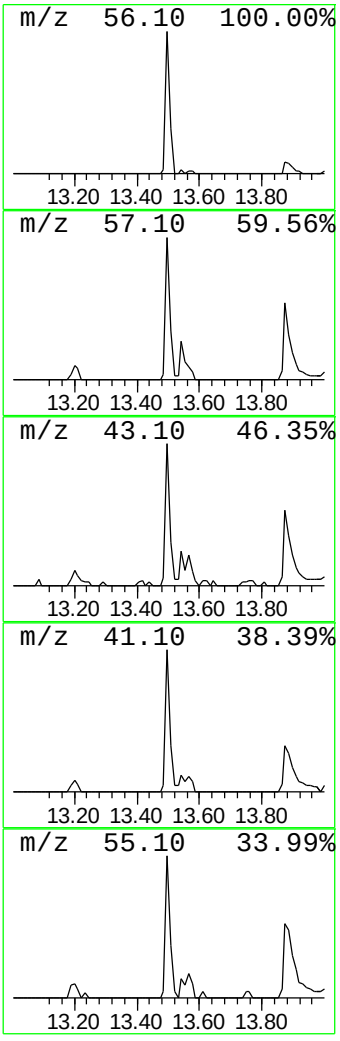
****

Peak Number 9 unknown13.50 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.50	3.08 ng	131033	Chrysene-d12	14.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclobutane, 1-hexyl-2,3-dimethyl-	168	C12H24	055170-84-8	38
2	Hexane, 3,4-dimethyl-	114	C8H18	000583-48-2	38
3	Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	38
4	Urea, N,N'-di-2-propenyl-	140	C7H12N2O	001801-72-5	38
5	2-Methyl-n-1-tridecene	196	C14H28	018094-01-4	38





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Sample : H3379-13
Misc :
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Instrument : BNA_F
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

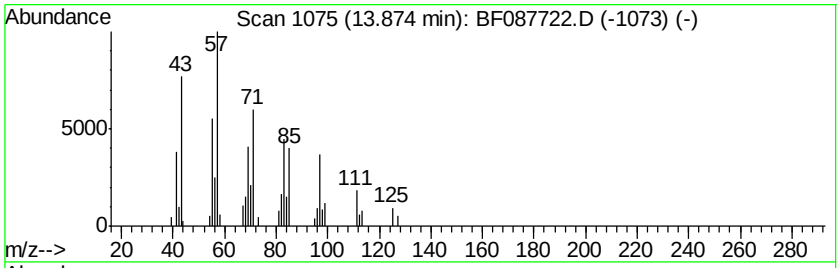
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

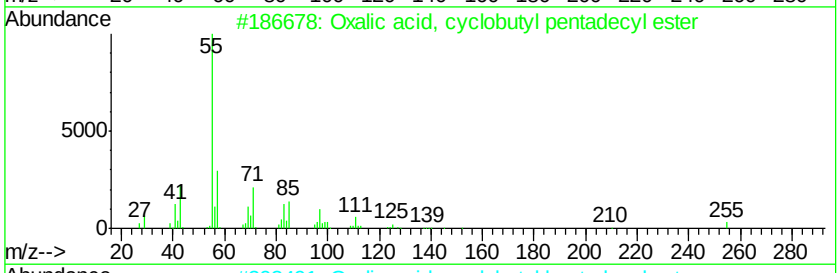
****

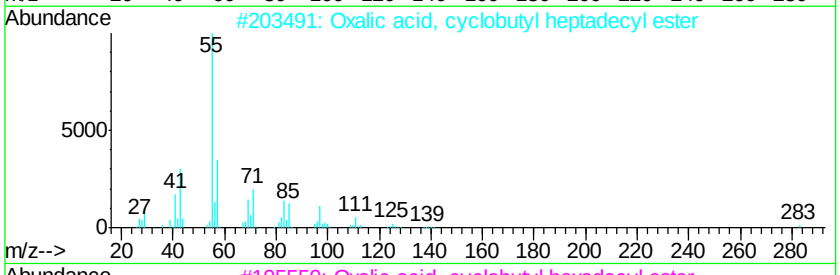
Peak Number 10 Oxalic acid, cyclobutyl pen... Concentration Rank 10

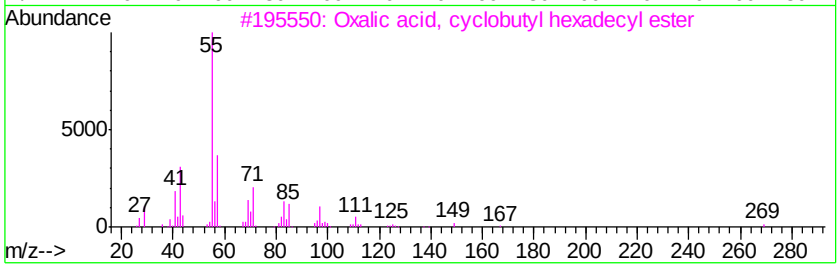
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	2.52 ng	107114	Chrysene-d12	14.01

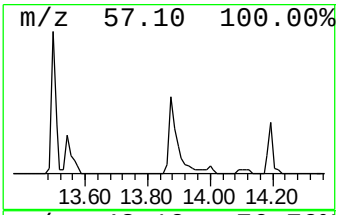
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxalic acid, cyclobutyl pentadec...	354	C21H38O4	1000309-70-5	91
2	Oxalic acid, cyclobutyl heptadec...	382	C23H42O4	1000309-70-7	91
3	Oxalic acid, cyclobutyl hexadecy...	368	C22H40O4	1000309-70-6	90
4	Oxalic acid, cyclobutyl tetradec...	340	C20H36O4	1000309-70-9	72
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	70

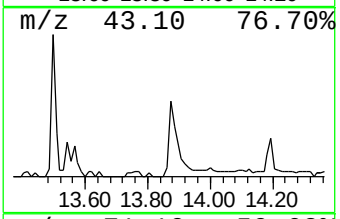


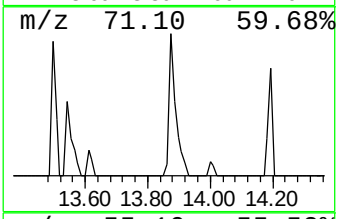


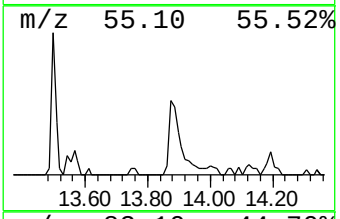


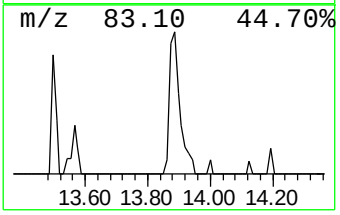












Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060516\
Data File : BF087722.D
Acq On : 5 Jun 2016 22:22
Operator : UM/SJ
Sample : H3379-13
Misc :
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Instrument : BNA_F
ClientSampleId : SB-4

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Propane, 2,2-dime...	1.76	229.8	ng	7846660	1	6.86	682774	20.0
Propane, 1,1-dime...	2.15	9.8	ng	334267	1	6.86	682774	20.0
(S)-(+)-1,2-Propa...	3.21	2.9	ng	100340	1	6.86	682774	20.0
2-Pentanone, 4-hy...	5.05	8.8	ng	300144	1	6.86	682774	20.0
unknown6.63	6.63	88.6	ng	3025970	1	6.86	682774	20.0
Hexadecanoic acid...	12.80	4.8	ng	205412	5	14.01	851534	20.0
unknown13.50	13.50	3.1	ng	131033	5	14.01	851534	20.0
Oxalic acid, cycl...	13.87	2.5	ng	107114	5	14.01	851534	20.0