LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG061019\
Data File : BG041162.D
Acq On : 10 Jun 2019 12:56
Operator : HP/JU
Sample : K3223-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : DUP-0532-190605

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:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG052919.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	3.183	12	16	28	rVB	194112	290331	7.24%	1.284%
2	3.435	53	59	78	rVB	2472342	4010736	100.00%	17.739%
3	5.639	427	434	446	rBV	381616	626047	15.61%	2.769%
4	5.762	448	455	465	rVV	520662	852445	21.25%	3.770%
5	7.248	701	708	718	rBV	286865	494417	12.33%	2.187%
6	7.630	765	773	783	rBV	911167	1584072	39.50%	7.006%
7	8.047	839	844	849	rBV2	40435	68316	1.70%	0.302%
8	8.106	849	854	861	rVB	151057	259599	6.47%	1.148%
9	8.429	901	909	919	rBV	629143	1095319	27.31%	4.844%
10	9.281	1045	1054	1064	rBV	553074	1029422	25.67%	4.553%
11	10.926	1326	1334	1348	rBV2	219972	449032	11.20%	1.986%
12	11.796	1470	1482	1495	rBV	83577	182511	4.55%	0.807%
13	13.359	1739	1748	1762	rBV	1661412	2545405	63.46%	11.258%
14	14.734	1975	1982	1991	rBV2	348633	568009	14.16%	2.512%
15	16.220	2229	2235	2245	rBV	1241223	1893729	47.22%	8.376%
16	17.478	2441	2449	2462	rBV	460653	722264	18.01%	3.194%
17	18.335	2587	2595	2606	rBV2	82178	153456	3.83%	0.679%
18	19.599	2805	2810	2819	rBV5	35198	65021	1.62%	0.288%
19	20.075	2885	2891	2901	rBV	2925724	3795381	94.63%	16.786%
20	21.350	3102	3108	3116	rBV4	59807	111132	2.77%	0.492%
21	21.755	3170	3177	3185	rBV2	492954	838655	20.91%	3.709%
22	22.519	3302	3307	3312	rBV3	29658	52379	1.31%	0.232%
23	23.224	3422	3427	3434	rVB4	30393	58052	1.45%	0.257%
24	24.046	3561	3567	3576	rVB3	31575	72644	1.81%	0.321%
25	25.086	3734	3744	3755	rVB	241022	751788	18.74%	3.325%
26	27.589	4159	4170	4172	rBV10	13710	40161	1.00%	0.178%

Sum of corrected areas: 22610323

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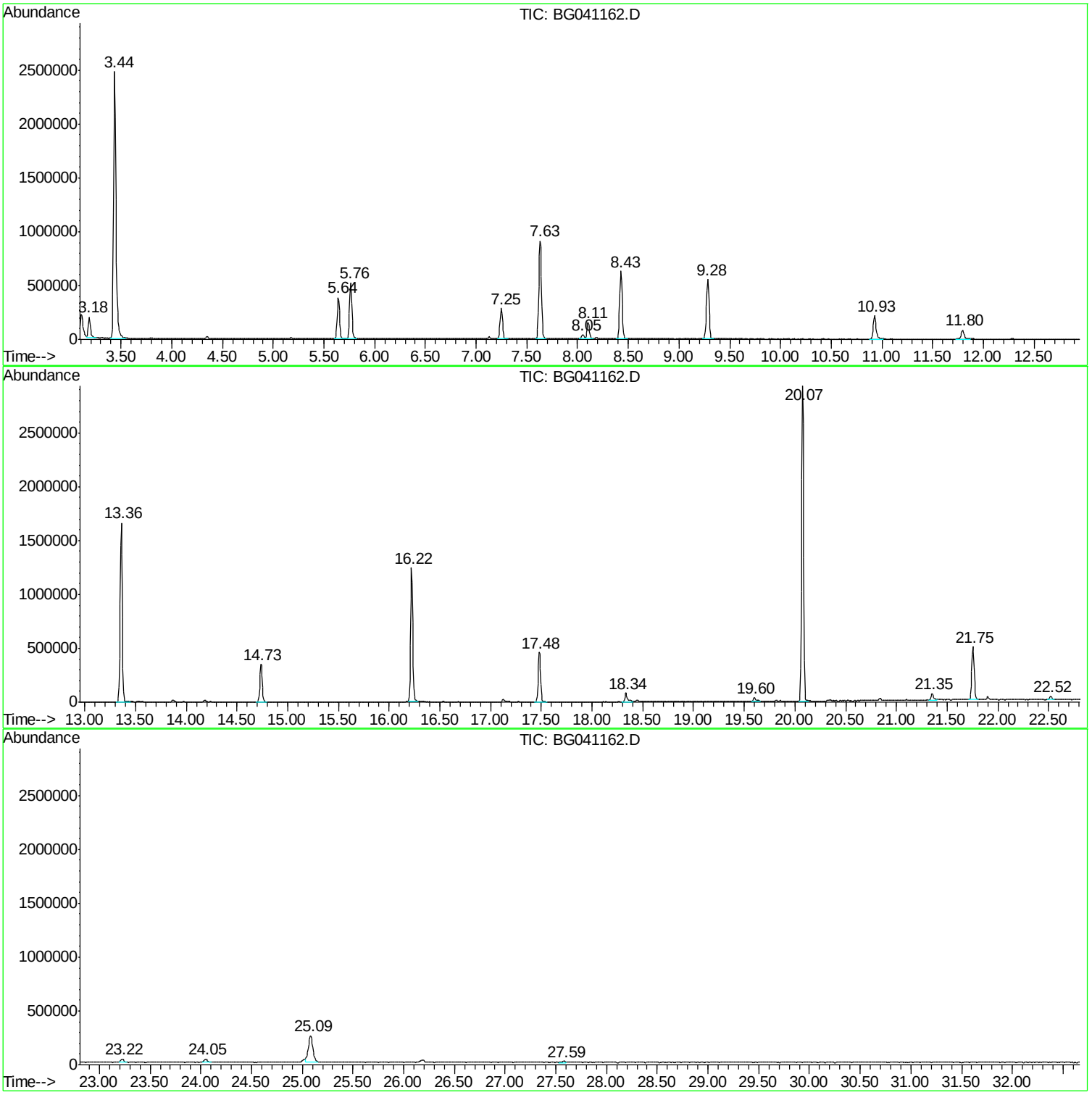
Instrument :
BNA_G
ClientSampleId :
DUP-0532-190605

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG052919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG061019\
Data File : BG041162.D
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Operator : HP/JU
Sample : K3223-03
Misc :
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Instrument : BNA_G
ClientSampleId : DUP-0532-190605

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG052919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

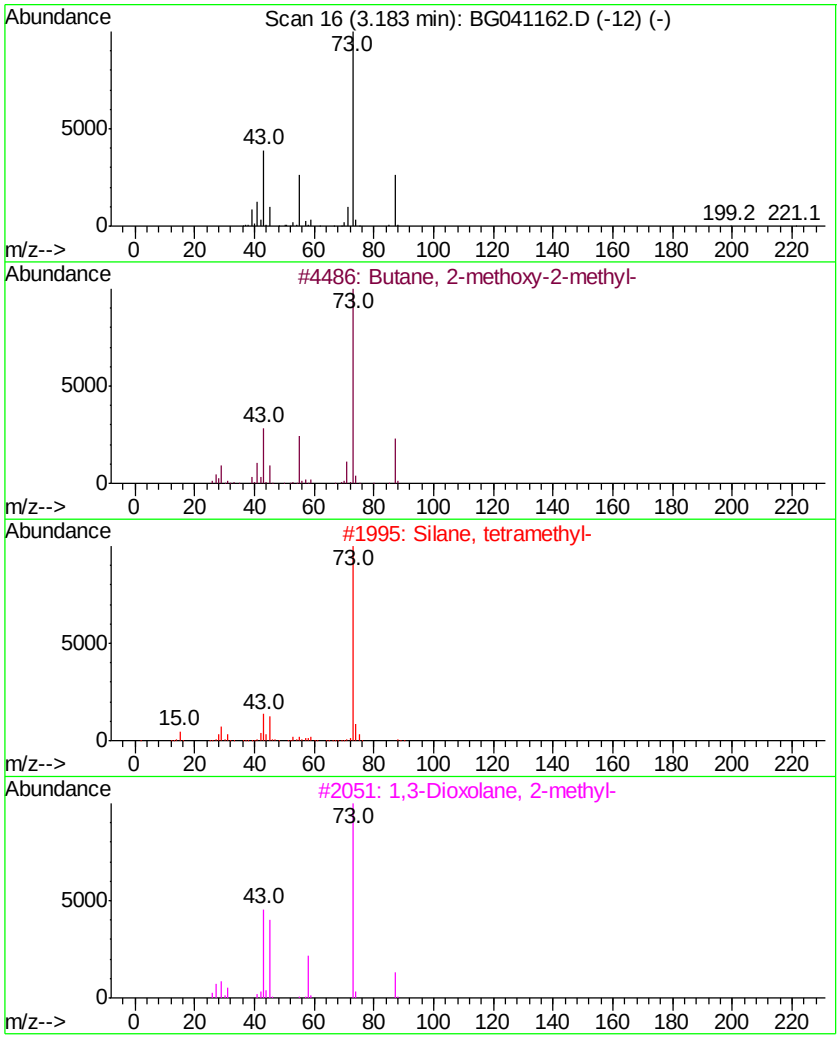
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

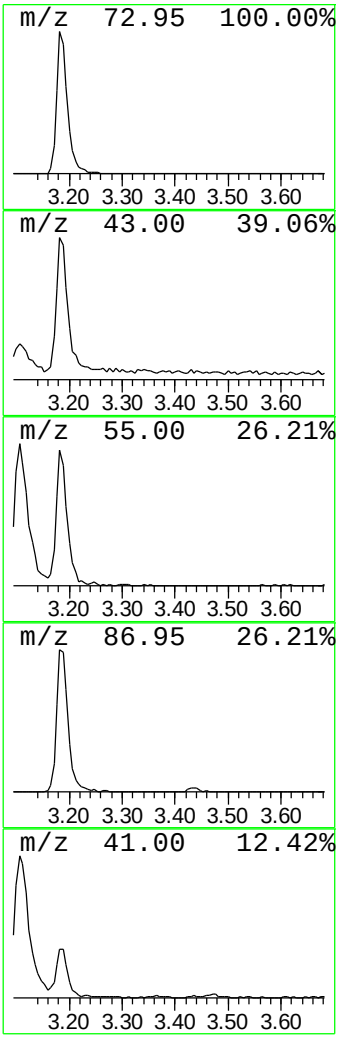
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.18	22.37 ng	290331	1,4-Dichlorobenzene-d4	8.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
4	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	9





Library Search Compound Report

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Data File : BG041162.D
Acq On : 10 Jun 2019 12:56
Operator : HP/JU
Sample : K3223-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : DUP-0532-190605

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG052919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

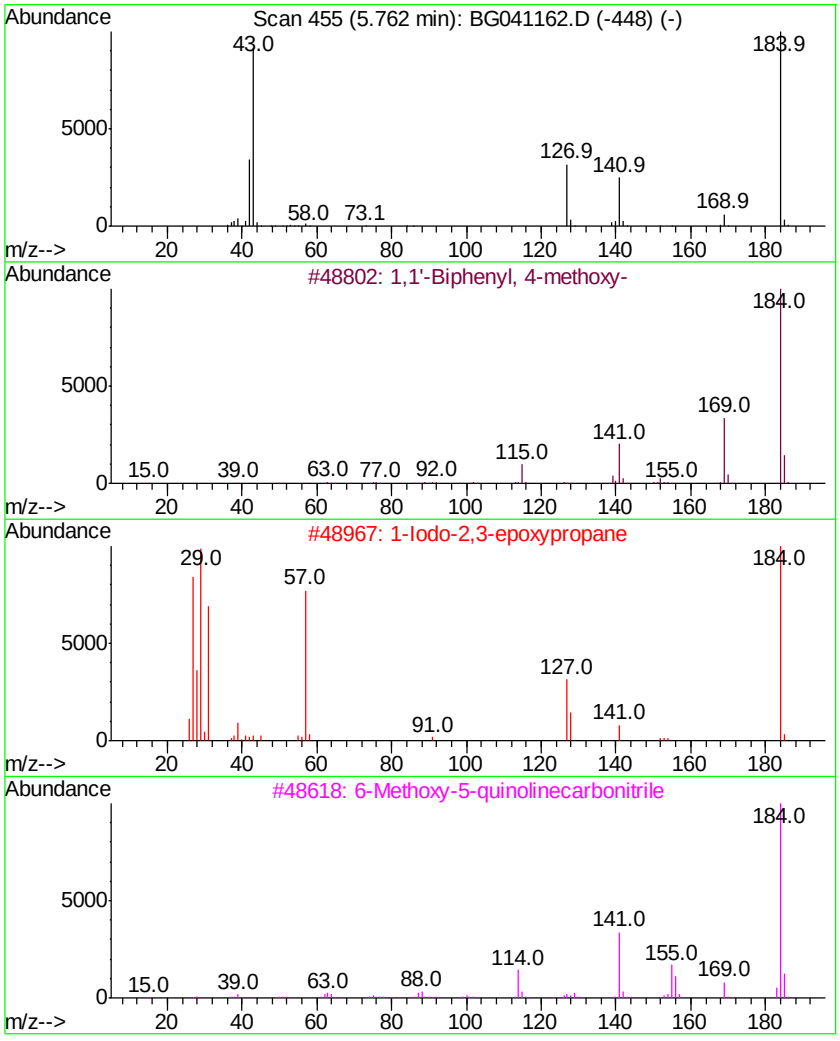
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

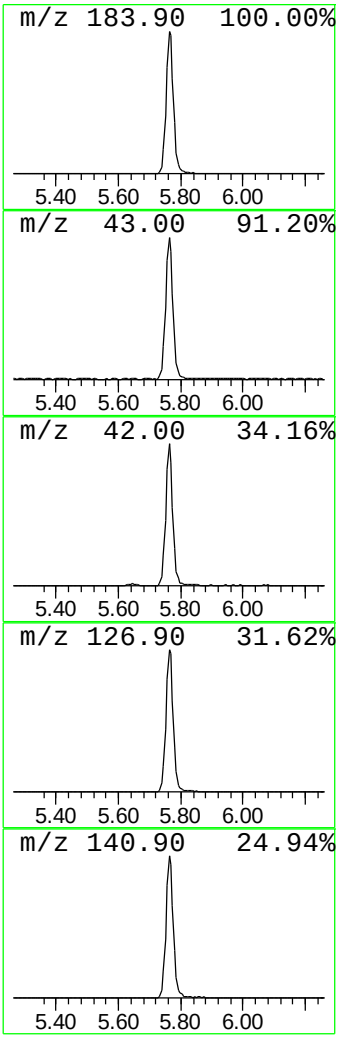
****

Peak Number 3 unknown5.76 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.76	65.67 ng	852445	1,4-Dichlorobenzene-d4	8.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1'-Biphenyl, 4-methoxy-	184	C13H12O	000613-37-6	38
2	1-Iodo-2,3-epoxypropane	184	C3H5IO	000624-57-7	28
3	6-Methoxy-5-quinolinecarbonitrile	184	C11H8N2O	087299-97-6	28
4	Propyl octanoate	186	C11H22O2	000624-13-5	22
5	1,1'-Biphenyl, 2-methoxy-	184	C13H12O	000086-26-0	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG061019\
Data File : BG041162.D
Acq On : 10 Jun 2019 12:56
Operator : HP/JU
Sample : K3223-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : DUP-0532-190605

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG052919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

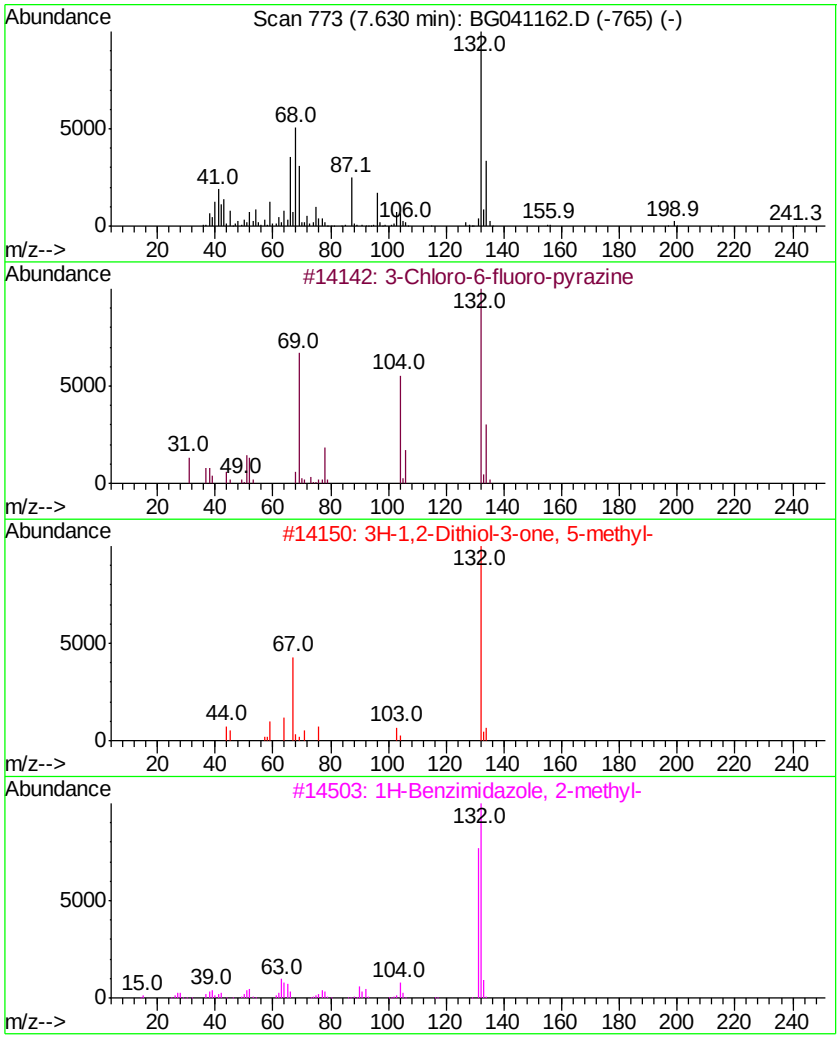
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

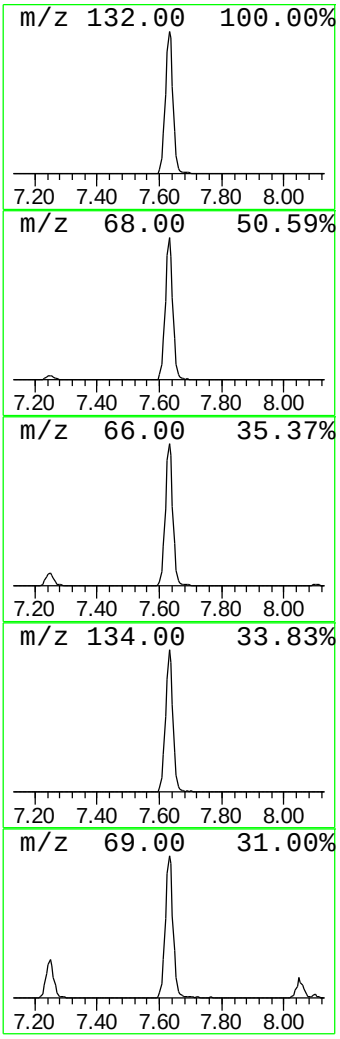
****

Peak Number 4 unknown7.63 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.63	122.04 ng	1584070	1,4-Dichlorobenzene-d4	8.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	22
2	3H-1,2-Dithiol-3-one, 5-methyl-	132	C4H4OS2	003620-08-4	22
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	18
4	5-Aminoindole	132	C8H8N2	005192-03-0	14
5	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	14





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG061019\
Data File : BG041162.D
Acq On : 10 Jun 2019 12:56
Operator : HP/JU
Sample : K3223-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : DUP-0532-190605

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG052919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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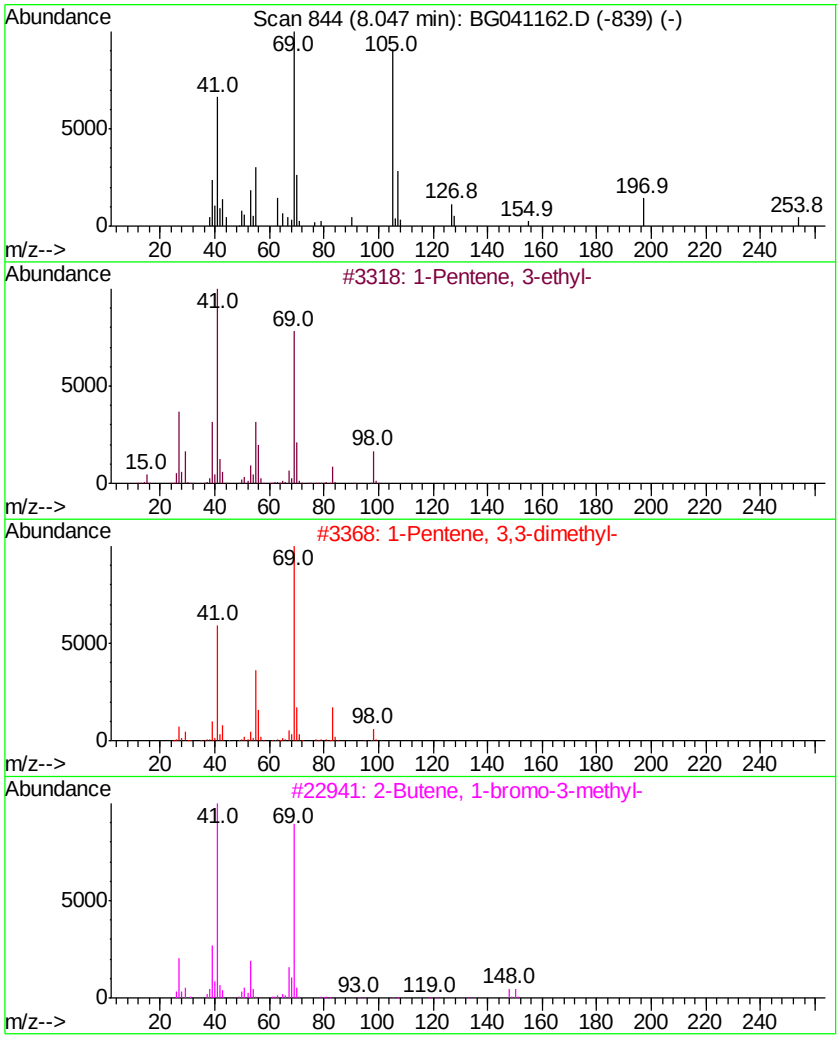
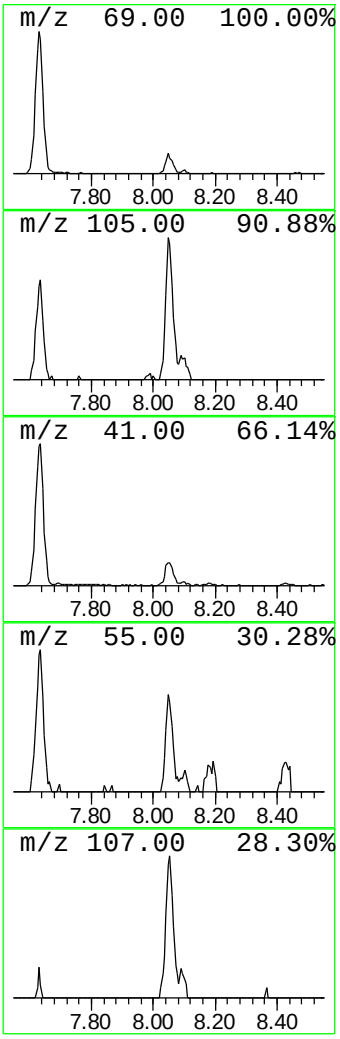
****

Peak Number 5 unknown8.05 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.05	5.26 ng	68316	1,4-Dichlorobenzene-d4	8.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentene, 3-ethyl-	98	C7H14	004038-04-4	25
2	1-Pentene, 3,3-dimethyl-	98	C7H14	003404-73-7	23
3	2-Butene, 1-bromo-3-methyl-	148	C5H9Br	000870-63-3	17
4	Cyanamide, dimethyl-	70	C3H6N2	001467-79-4	17
5	4-Chlorobutyric acid, 2-pentyl e...	192	C9H17ClO2	1000357-76-6	10





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG061019\
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Acq On : 10 Jun 2019 12:56
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Sample : K3223-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : DUP-0532-190605

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG052919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

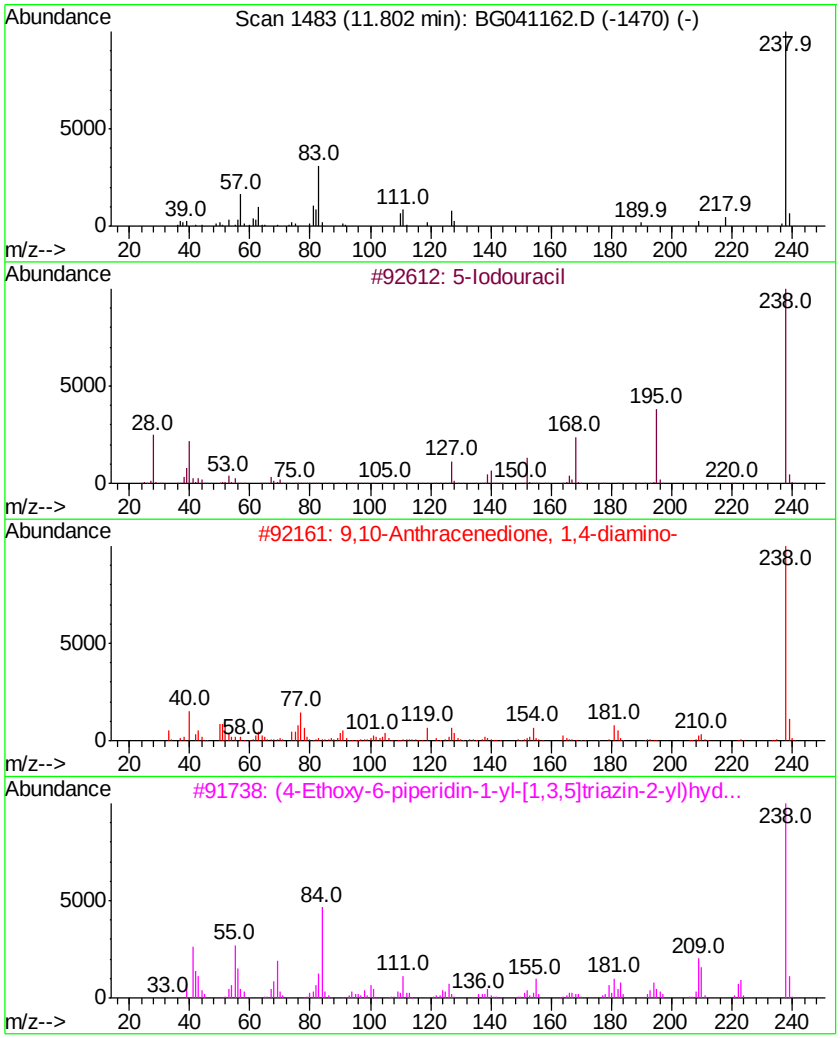
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

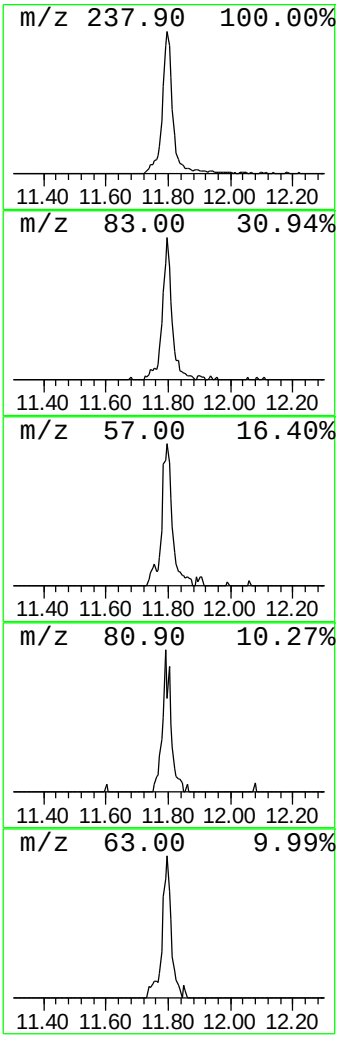
****

Peak Number 7 unknown11.80 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.80	8.13 ng	182511	Naphthalene-d8	10.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Iodouracil	238	C4H3IN2O2	000696-07-1	37
2	9,10-Anthracenedione, 1,4-diamino-	238	C14H10N2O2	000128-95-0	9
3	(4-Ethoxy-6-piperidin-1-yl-[1,3,...	238	C10H18N6O	1000302-56-6	9
4	Imidazo[4,5-e][1,4]diazepine-5,8...	238	C10H14N4O3	077246-18-5	9
5	9,10-Anthracenedione, 1,2-diamino-	238	C14H10N2O2	001758-68-5	9





Library Search Compound Report

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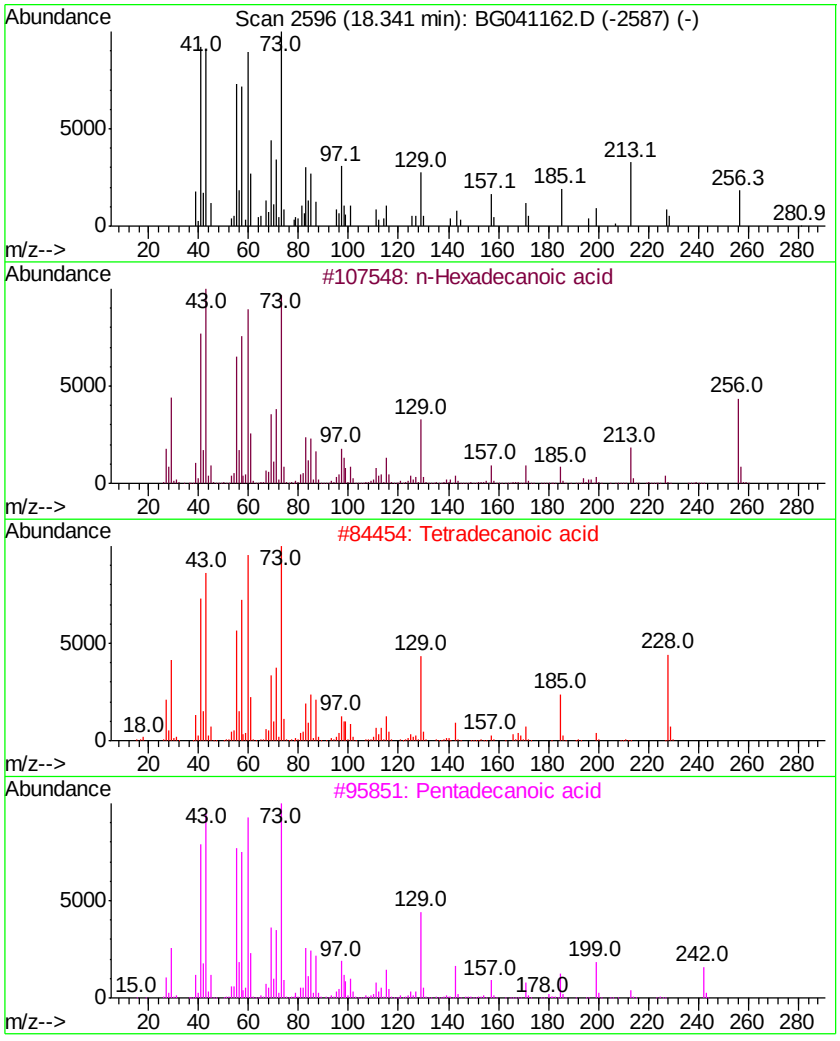
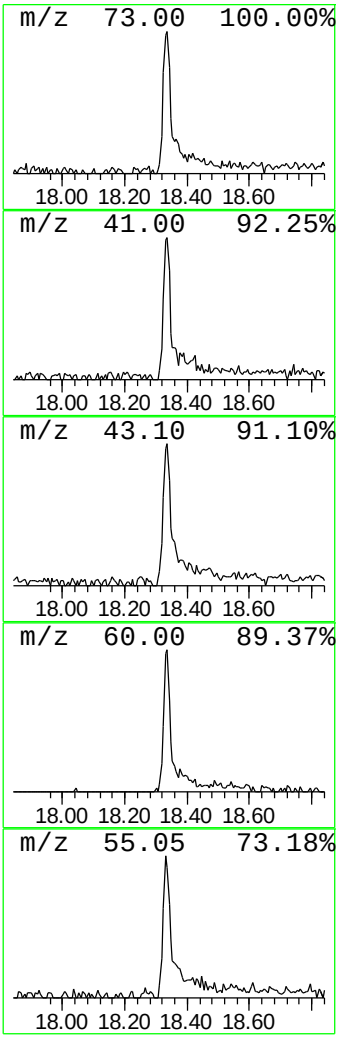
****

Peak Number 8 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.34	4.25 ng	153456	Phenanthrene-d10	17.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	72
4	Tridecanoic acid	214	C13H26O2	000638-53-9	64
5	n-Decanoic acid	172	C10H20O2	000334-48-5	53





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

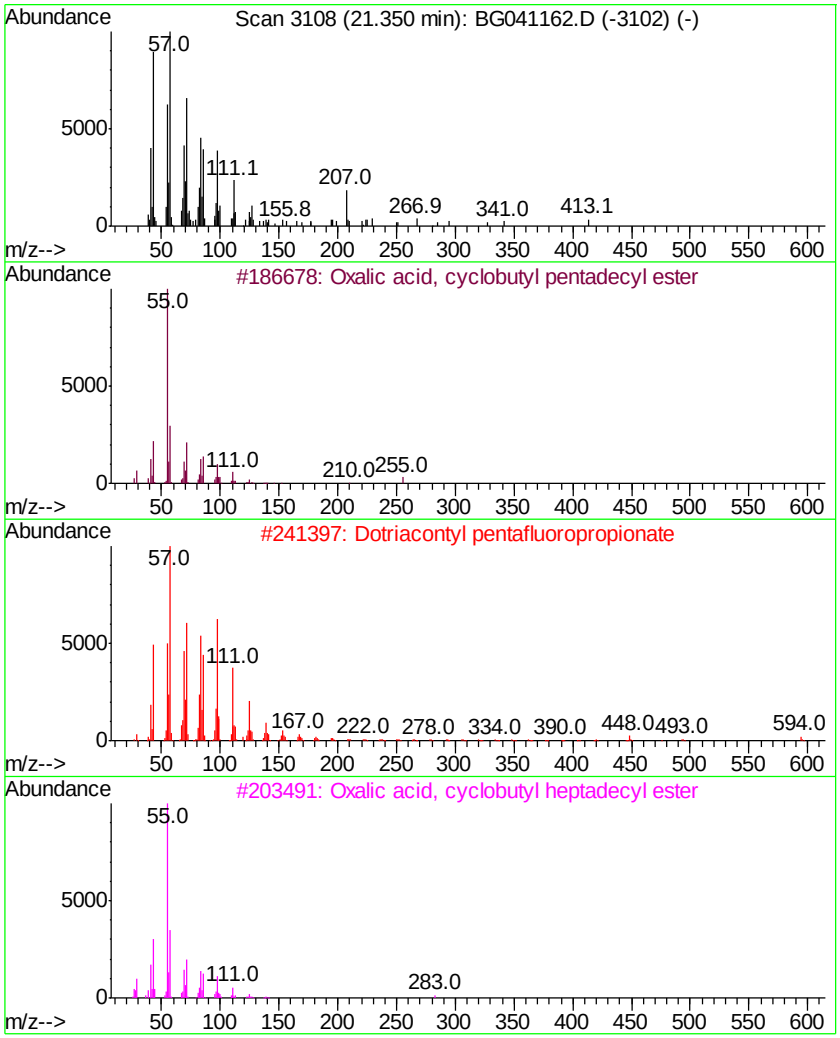
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

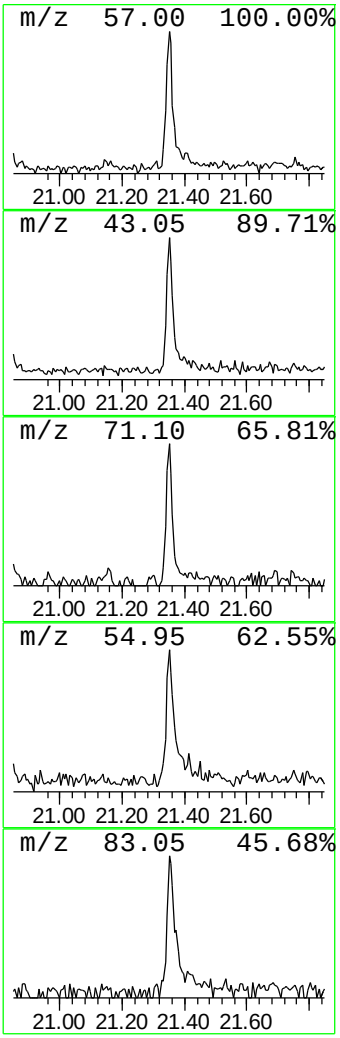
****

Peak Number 9 Oxalic acid, cyclobutyl pen... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.35	2.65 ng	111132	Chrysene-d12	21.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxalic acid, cyclobutyl pentadec...	354	C21H38O4	1000309-70-5	87
2	Dotriacontyl pentafluoropropionate	612	C35H65F5O2	1000351-81-4	87
3	Oxalic acid, cyclobutyl heptadec...	382	C23H42O4	1000309-70-7	87
4	Cyclohexadecane	224	C16H32	000295-65-8	86
5	Oxalic acid, isobutyl octadecyl ...	398	C24H46O4	1000309-38-3	83





Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-methoxy...	3.18	22.4	ng	290331	1	8.11	259599	20.0
unknown5.76	5.76	65.7	ng	852445	1	8.11	259599	20.0
unknown7.63	7.63	122.0	ng	1584070	1	8.11	259599	20.0
unknown8.05	8.05	5.3	ng	68316	1	8.11	259599	20.0
unknown11.80	11.80	8.1	ng	182511	2	10.93	449032	20.0
n-Hexadecanoic acid	18.34	4.3	ng	153456	4	17.48	722264	20.0
Oxalic acid, cycl...	21.35	2.6	ng	111132	5	21.75	838655	20.0