LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG050919\
Data File : BG040839.D
Acq On : 10 May 2019 7:08
Operator : HP/JU
Sample : K2764-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : P021-SS008-1218-01

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-BG042319.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	3.153	4	11	19	rBV	118675	213254	4.77%	0.838%
2	3.229	19	24	35	rVB	218739	299465	6.69%	1.177%
3	5.674	431	440	451	rBV	1083325	1714179	38.31%	6.735%
4	7.278	705	713	724	rBV	1203643	2103500	47.01%	8.265%
5	7.665	771	779	788	rBV	1118768	1891168	42.26%	7.431%
6	8.141	853	860	868	rBV	194090	330436	7.38%	1.298%
7	8.464	907	915	924	rBV	769578	1323505	29.58%	5.200%
8	9.316	1053	1060	1068	rBV	738806	1312158	29.32%	5.156%
9	10.961	1331	1340	1349	rVB	258183	463120	10.35%	1.820%
10	13.394	1747	1754	1762	rBV	1846599	2768667	61.87%	10.878%
11	14.211	1887	1893	1899	rBV	295202	414632	9.27%	1.629%
12	14.769	1982	1988	1995	rBV2	475524	749093	16.74%	2.943%
13	16.255	2234	2241	2263	rBV	1832293	2835297	63.36%	11.140%
14	17.513	2449	2455	2469	rBV2	706074	1047772	23.41%	4.117%
15	18.365	2593	2600	2607	rBV2	232009	333523	7.45%	1.310%
16	19.628	2810	2815	2823	rBV2	86116	145843	3.26%	0.573%
17	20.110	2891	2897	2910	rBV	3348578	4474962	100.00%	17.583%
18	21.396	3110	3116	3130	rBV3	78614	225699	5.04%	0.887%
19	21.796	3177	3184	3194	rBV	642749	1114018	24.89%	4.377%
20	21.949	3206	3210	3217	rVB	40537	58407	1.31%	0.229%
21	22.577	3311	3317	3323	rBV	47329	80884	1.81%	0.318%
22	23.288	3433	3438	3446	rVB2	65037	120323	2.69%	0.473%
23	23.500	3466	3474	3480	rBV2	53777	108473	2.42%	0.426%
24	24.128	3573	3581	3588	rBV3	57174	129609	2.90%	0.509%
25	25.151	3739	3755	3769	rBV	305952	1106298	24.72%	4.347%
26	26.291	3942	3949	3959	rVB5	32563	86669	1.94%	0.341%

Sum of corrected areas: 25450954

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG050919\
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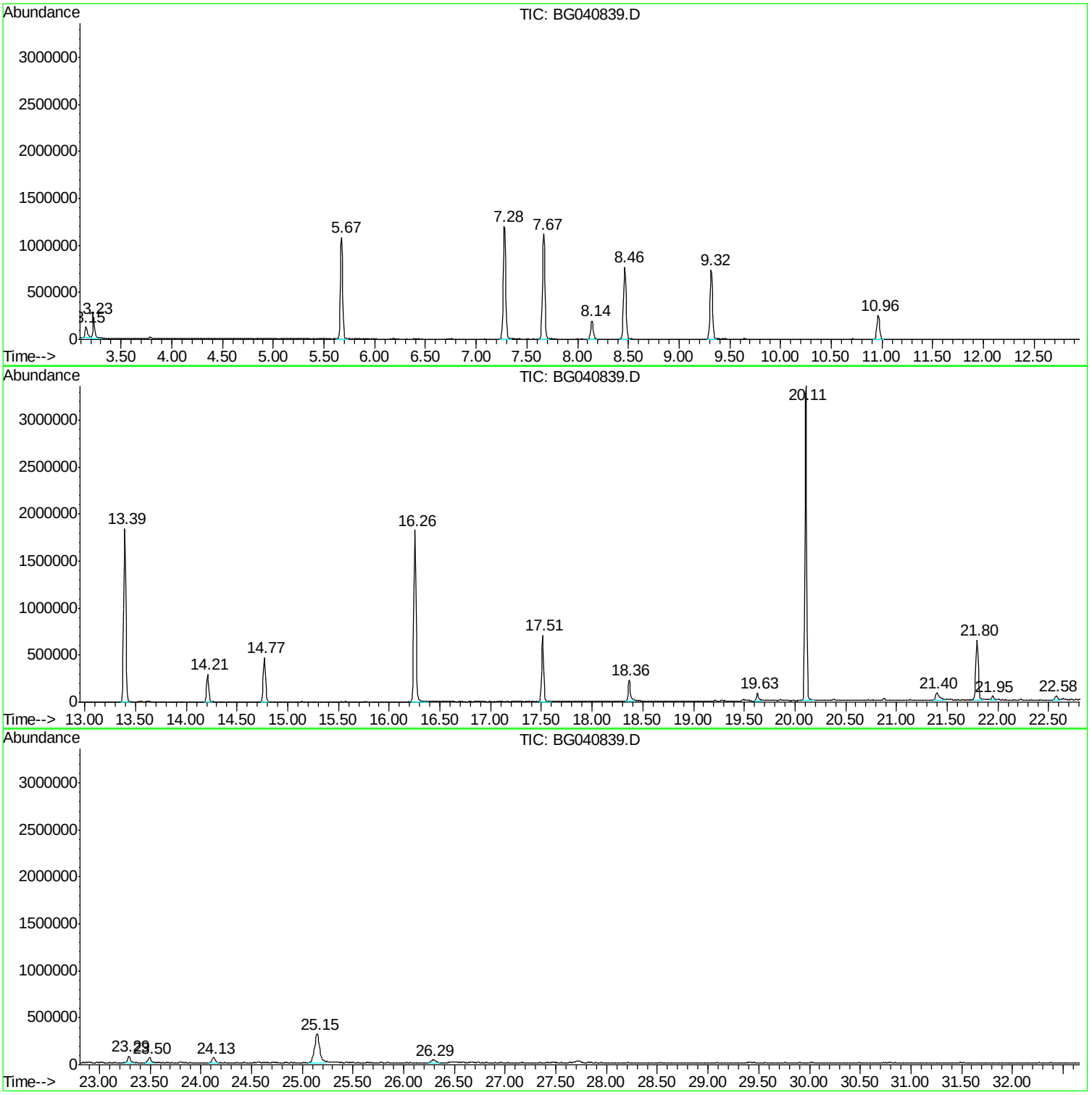
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
P021-SS008-1218-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG042319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG050919\
Data File : BG040839.D
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Operator : HP/JU
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Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : P021-SS008-1218-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG042319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

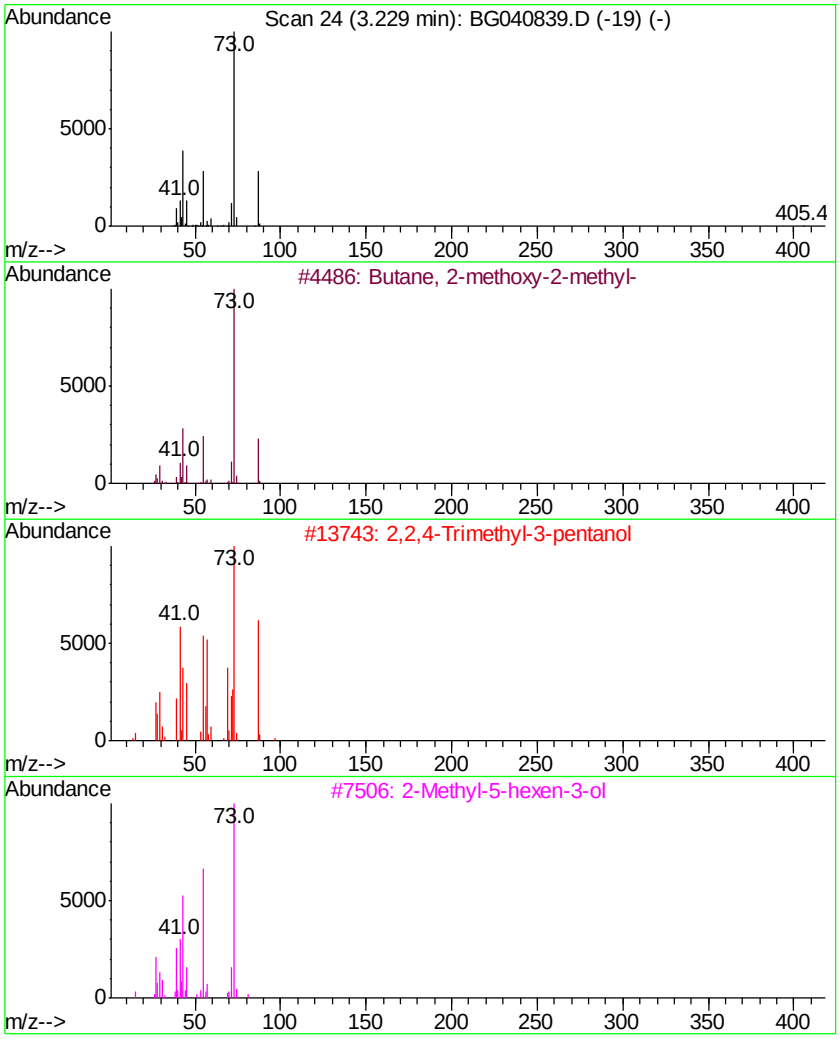
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

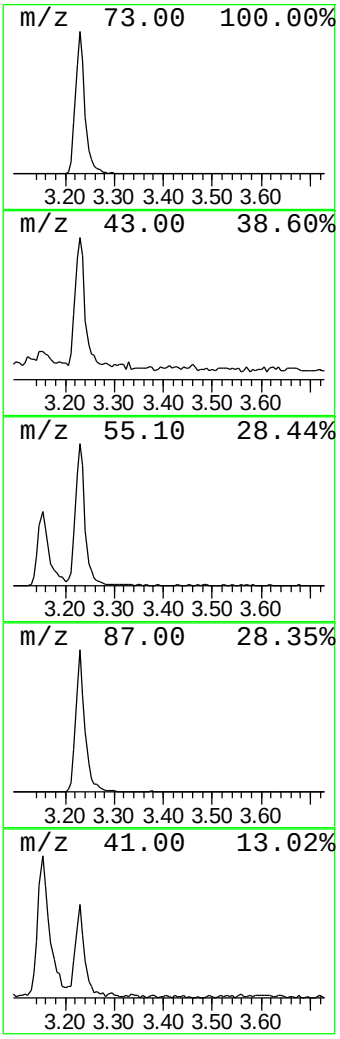
****

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.23	18.13 ng	299465	1,4-Dichlorobenzene-d4	8.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	42
3	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	16
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9





Library Search Compound Report

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Data File : BG040839.D
Acq On : 10 May 2019 7:08
Operator : HP/JU
Sample : K2764-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : P021-SS008-1218-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG042319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

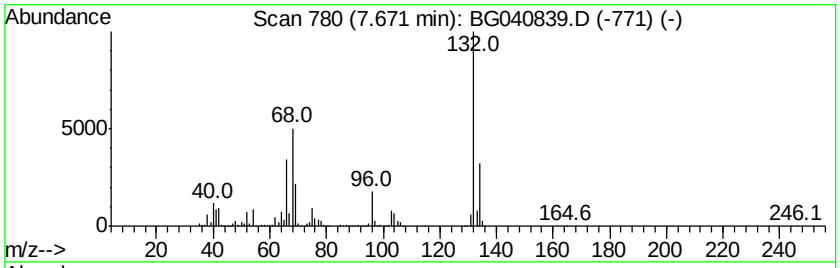
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

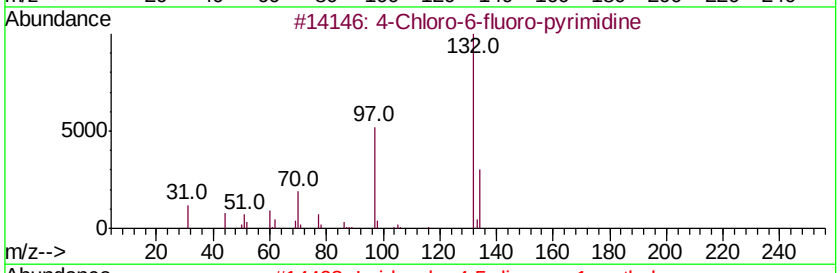
****

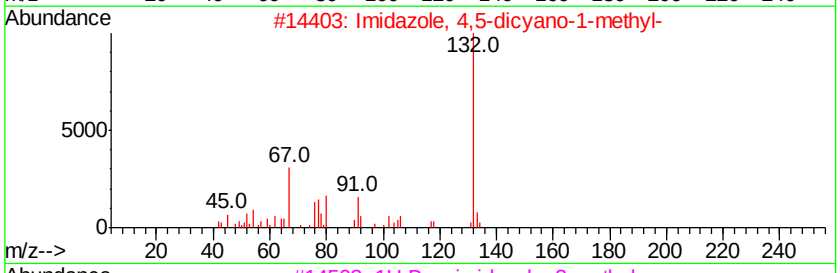
Peak Number 3 unknown7.67 Concentration Rank 1

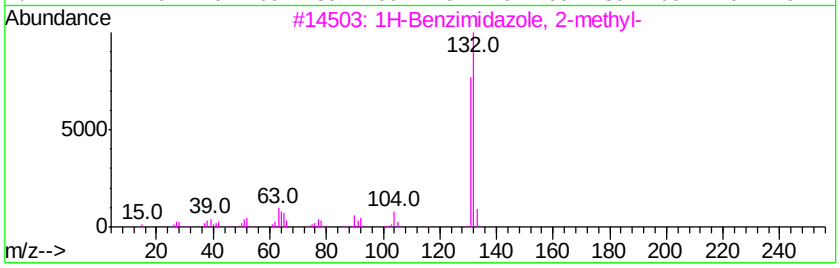
R.T.	EstConc	Area	Relative to ISTD	R.T.
7.67	114.47 ng	1891170	1,4-Dichlorobenzene-d4	8.14

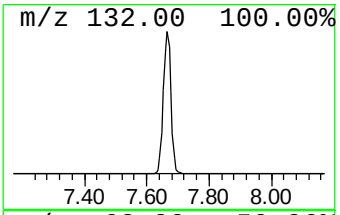
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	25
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4	5-Aminoindole	132	C8H8N2	005192-03-0	22
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16

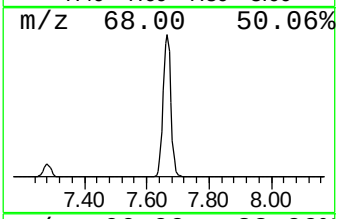


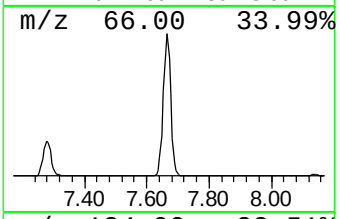


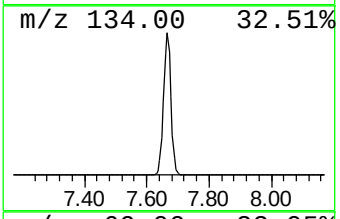


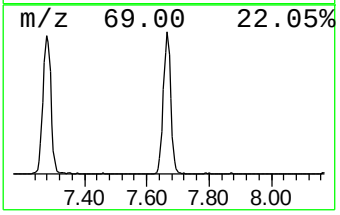












Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG050919\
Data File : BG040839.D
Acq On : 10 May 2019 7:08
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Sample : K2764-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : P021-SS008-1218-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG042319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

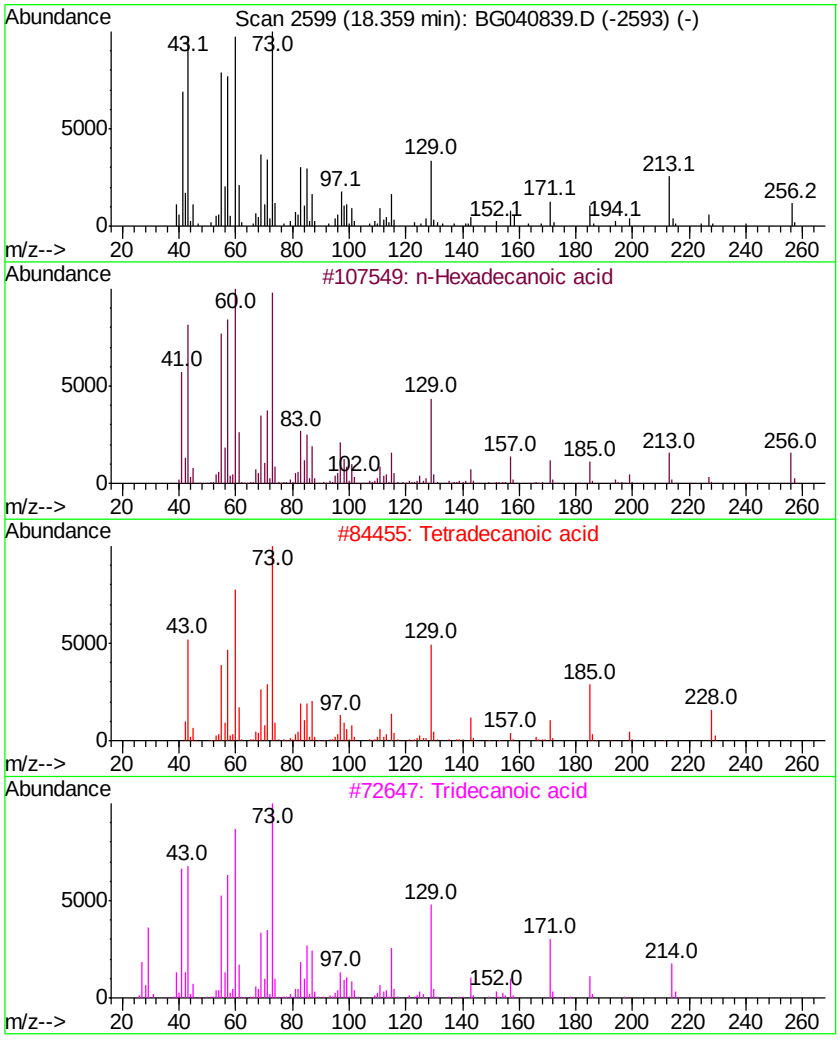
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

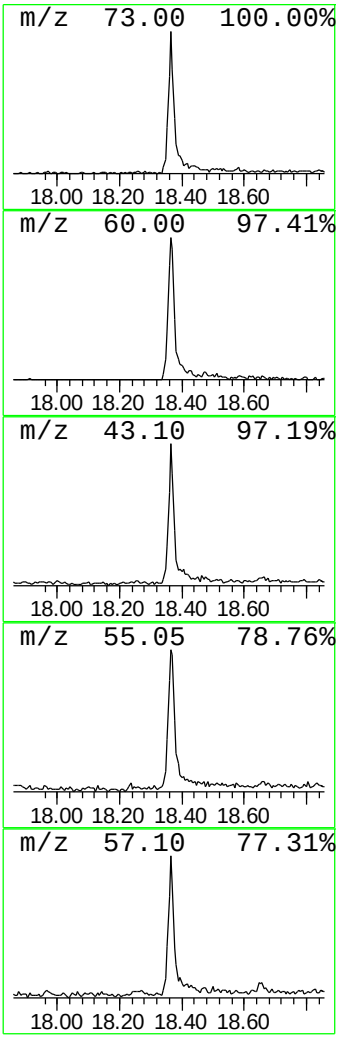
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.36	6.37 ng	333523	Phenanthrene-d10	17.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
3	Tridecanoic acid	214	C13H26O2	000638-53-9	89
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5	n-Decanoic acid	172	C10H20O2	000334-48-5	70





Library Search Compound Report

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Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : P021-SS008-1218-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG042319.M
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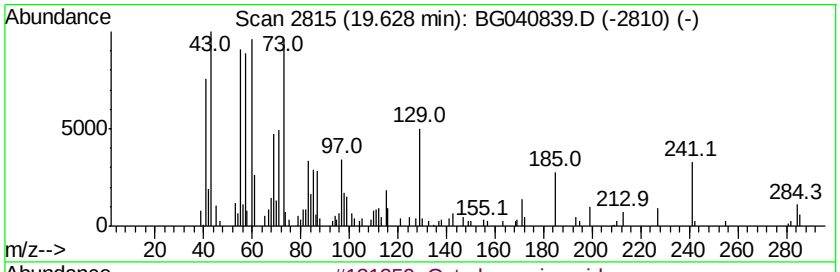
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

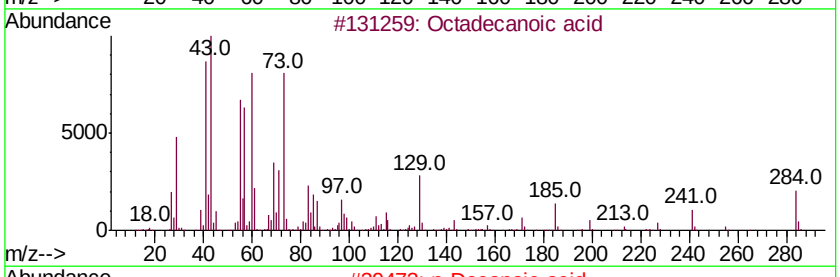
****

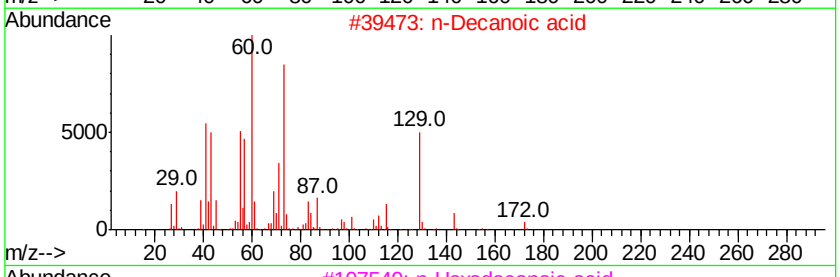
Peak Number 6 Octadecanoic acid Concentration Rank 7

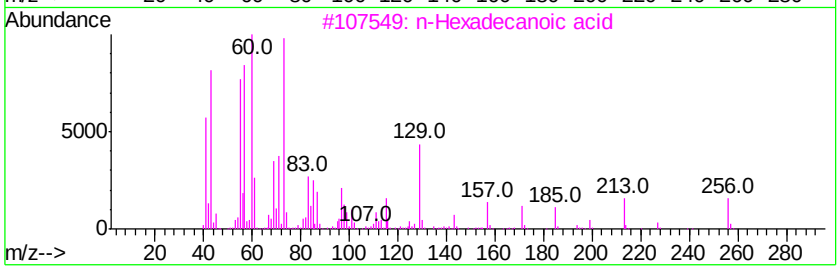
R.T.	EstConc	Area	Relative to ISTD	R.T.
19.63	2.78 ng	145843	Phenanthrene-d10	17.51

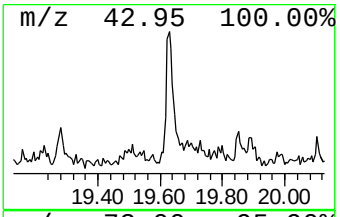
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	97
2	n-Decanoic acid	172	C10H20O2	000334-48-5	83
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	74
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	72
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	64

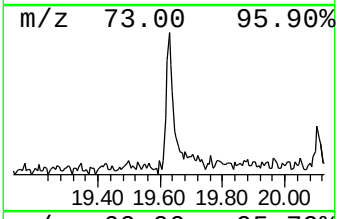


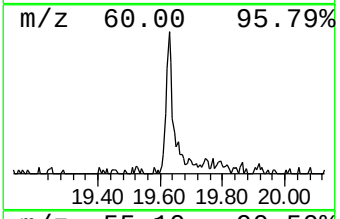


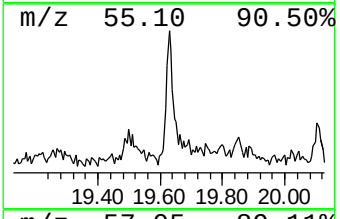


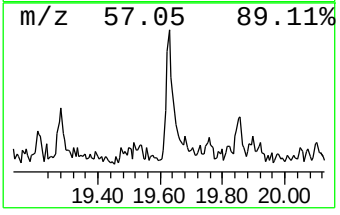












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Instrument : BNA_G
ClientSampleId : P021-SS008-1218-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG042319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

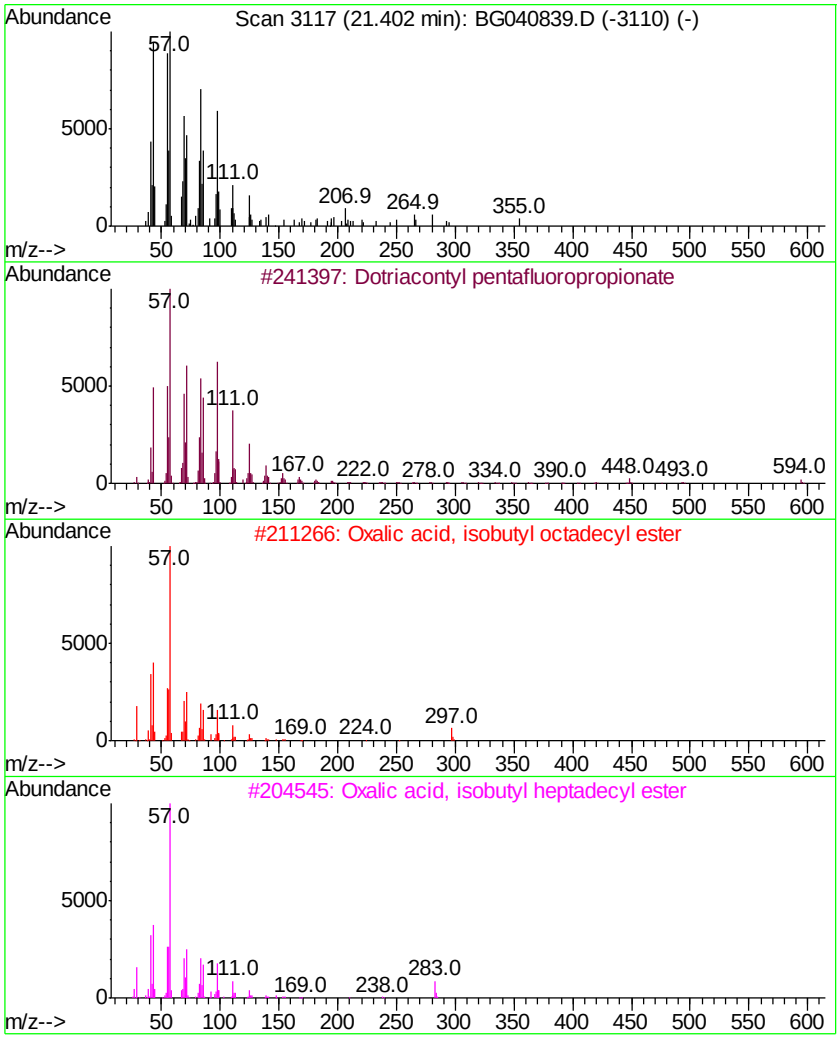
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

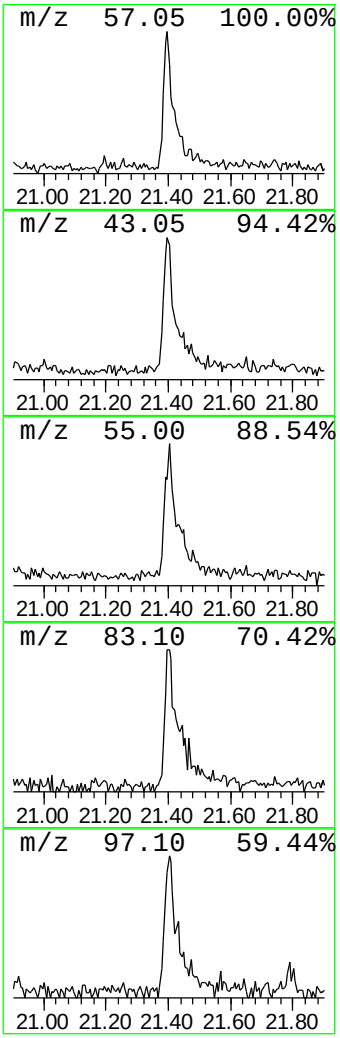
****

Peak Number 7 Dotriacontyl pentafluoropro... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.40	4.05 ng	225699	Chrysene-d12	21.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dotriacontyl pentafluoropropionate	612	C35H65F5O2	1000351-81-4	87
2	Oxalic acid, isobutyl octadecyl ...	398	C24H46O4	1000309-38-3	87
3	Oxalic acid, isobutyl heptadecyl...	384	C23H44O4	1000309-38-2	87
4	Dotriacontyl heptafluorobutyrate	662	C36H65F7O2	1000351-84-2	87
5	Dotriacontyl trifluoroacetate	562	C34H65F3O2	1000351-75-4	86





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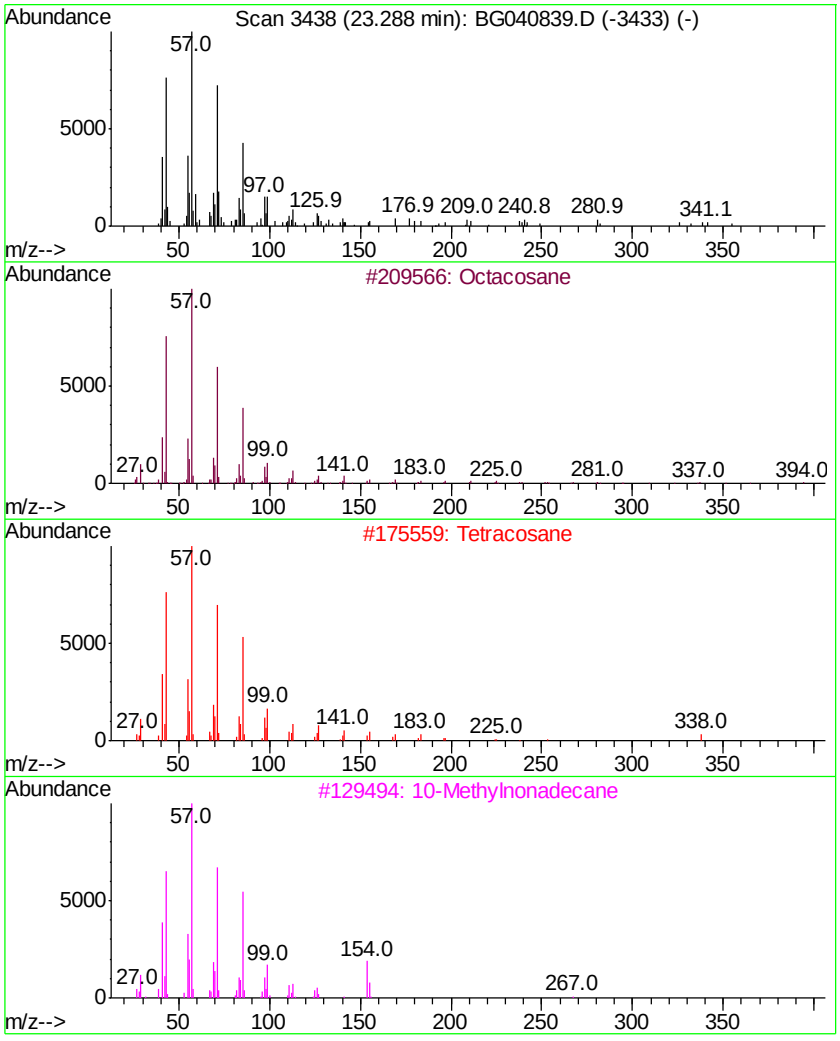
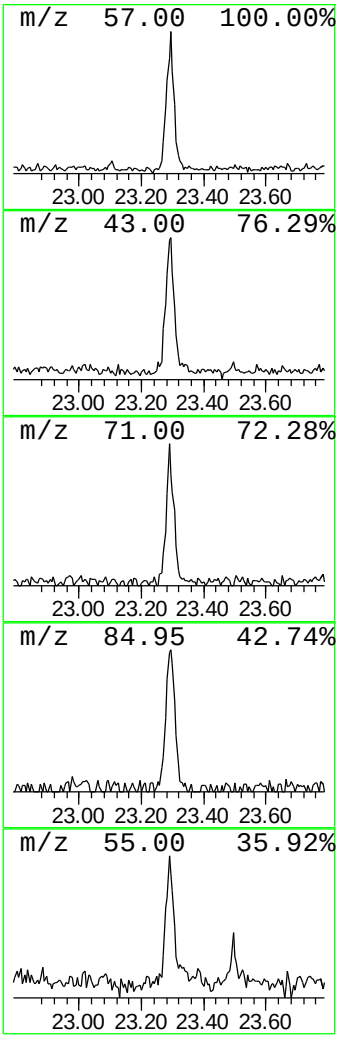
****

Peak Number 8 Octacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.29	2.16 ng	120323	Chrysene-d12	21.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	87
2	Tetracosane	338	C24H50	000646-31-1	81
3	10-Methylnonadecane	282	C20H42	056862-62-5	81
4	Hexacosane	366	C26H54	000630-01-3	81
5	Hexatriacontane	507	C36H74	000630-06-8	74





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Data File : BG040839.D
Acq On : 10 May 2019 7:08
Operator : HP/JU
Sample : K2764-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : P021-SS008-1218-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG042319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

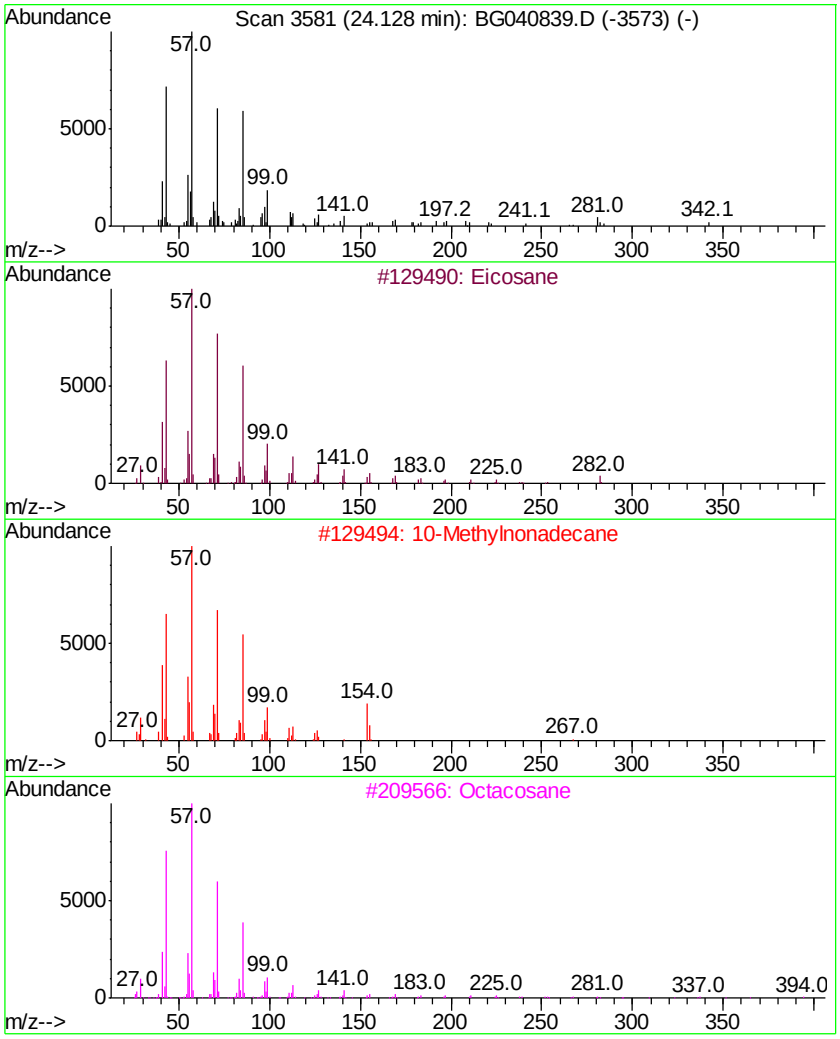
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

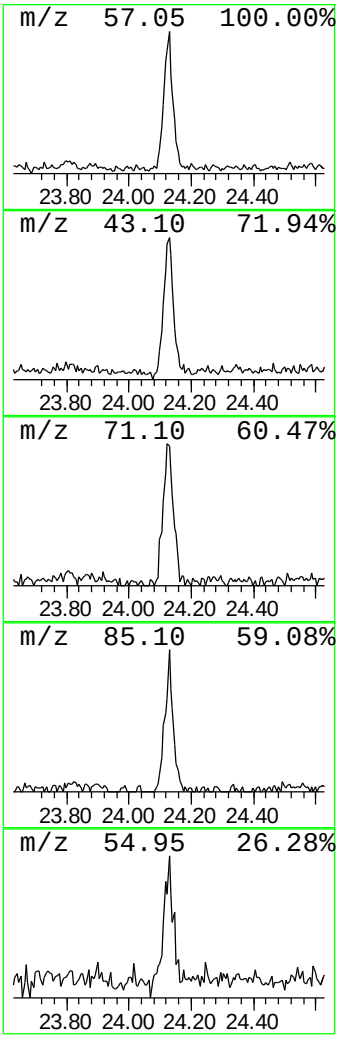
****

Peak Number 9 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.13	2.34 ng	129609	Perylene-d12	25.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	87
2	10-Methylnonadecane	282	C20H42	056862-62-5	80
3	Octacosane	394	C28H58	000630-02-4	68
4	Hexacosane	366	C26H54	000630-01-3	64
5	Tetracosane	338	C24H50	000646-31-1	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG050919\
Data File : BG040839.D
Acq On : 10 May 2019 7:08
Operator : HP/JU
Sample : K2764-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : P021-SS008-1218-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG042319.M
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
Butane, 2-methoxy...	3.23	18.1	ng	299465	1	8.14	330436	20.0
unknown7.67	7.67	114.5	ng	1891170	1	8.14	330436	20.0
n-Hexadecanoic acid	18.36	6.4	ng	333523	4	17.51	1047770	20.0
Octadecanoic acid	19.63	2.8	ng	145843	4	17.51	1047770	20.0
Dotriacontyl pent...	21.40	4.0	ng	225699	5	21.80	1114020	20.0
Octacosane	23.29	2.2	ng	120323	5	21.80	1114020	20.0
Eicosane	24.13	2.3	ng	129609	6	25.15	1106300	20.0