LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051623\
Data File : BG057439.D
Acq On : 16 May 2023 10:31
Operator : CG/JU
Sample : PB152548BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PB152548BL

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-BG042723.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG057439.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.391	309	315	324	rBV	149851	225500	10.58%	2.650%
2	5.879	391	398	408	rBV	381301	605231	28.40%	7.111%
3	7.506	667	675	689	rBV	387192	687498	32.26%	8.078%
4	8.364	814	821	829	rBB	67650	115503	5.42%	1.357%
5	9.545	1014	1022	1033	rBV	225621	414095	19.43%	4.866%
6	11.201	1297	1304	1311	rBV	99296	173361	8.14%	2.037%
7	13.604	1706	1713	1723	rBV	740834	1144836	53.73%	13.452%
8	14.978	1940	1947	1957	rVB	189632	297729	13.97%	3.498%
9	16.459	2193	2199	2218	rBV	631708	972688	45.65%	11.429%
10	17.716	2406	2413	2421	rBV	273423	423740	19.89%	4.979%
11	20.289	2845	2851	2856	rBV	1718638	2130905	100.00%	25.038%
12	22.028	3139	3147	3157	rBV	267797	458332	21.51%	5.385%
13	23.555	3401	3407	3414	rVB3	18203	34797	1.63%	0.409%
14	24.419	3549	3554	3561	rVB4	23364	49143	2.31%	0.577%
15	25.453	3721	3730	3735	rBV3	32517	87510	4.11%	1.028%
16	25.529	3735	3743	3756	rVB2	137518	415713	19.51%	4.885%
17	26.674	3929	3938	3947	rBV4	29973	87976	4.13%	1.034%
18	28.149	4180	4189	4205	rVB5	28699	107004	5.02%	1.257%
19	29.941	4482	4494	4508	rVB6	17504	79057	3.71%	0.929%

Sum of corrected areas: 8510618

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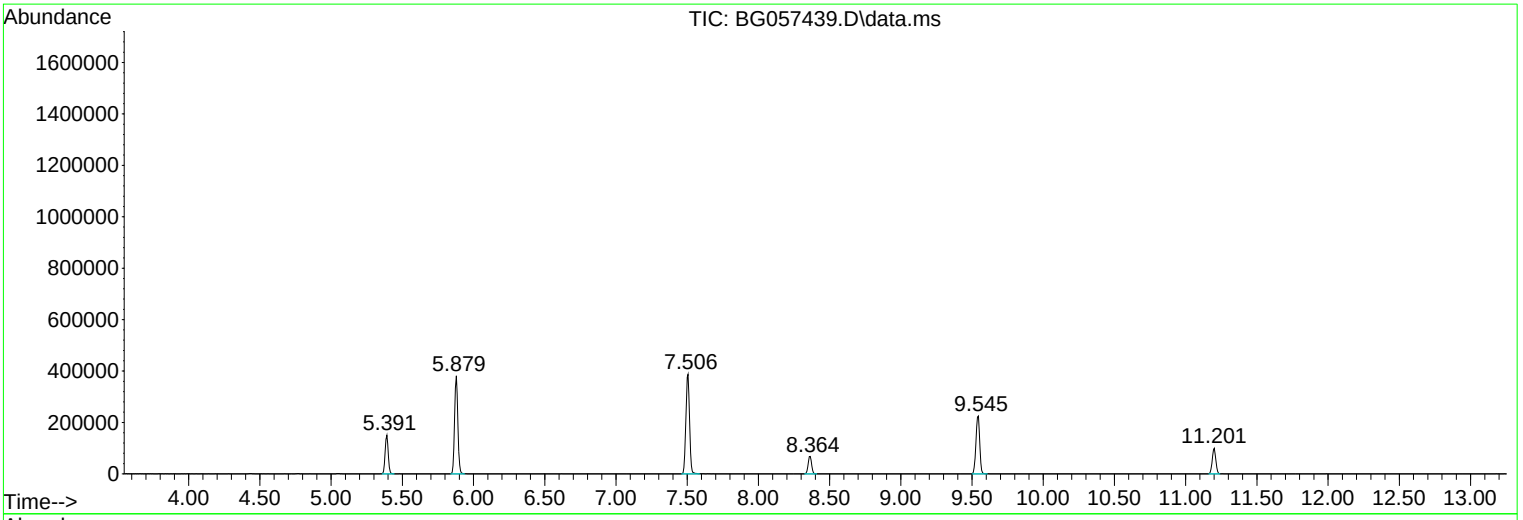
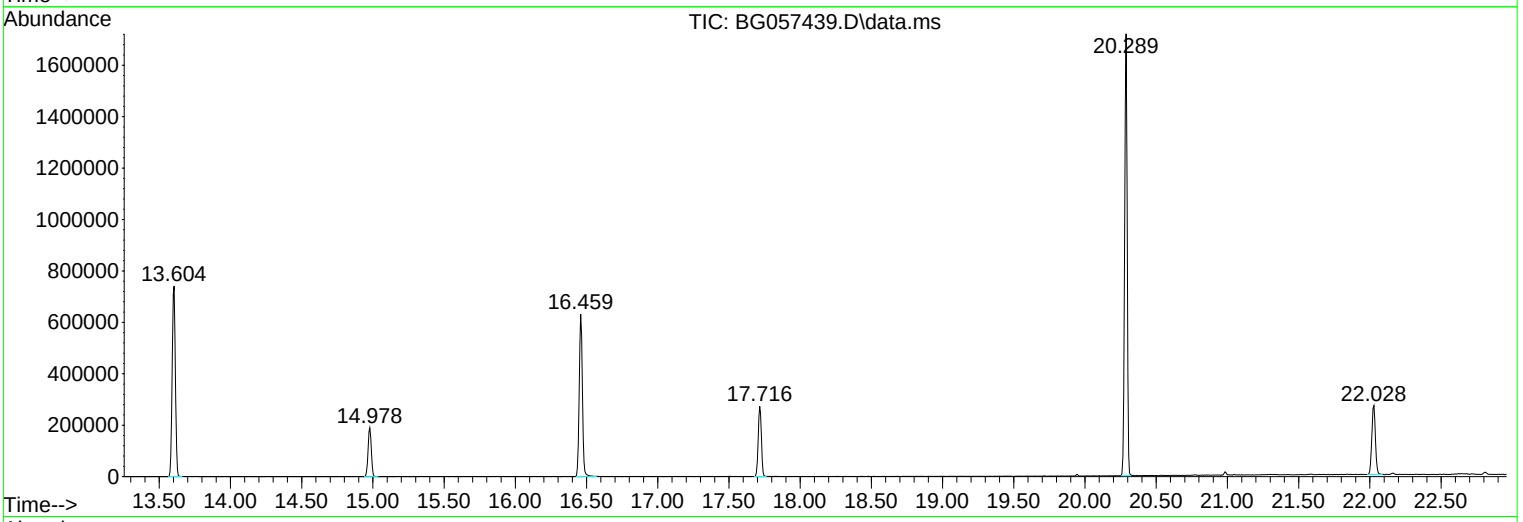
Misc :
ALS Vial : 3 Sample Multiplier: 1

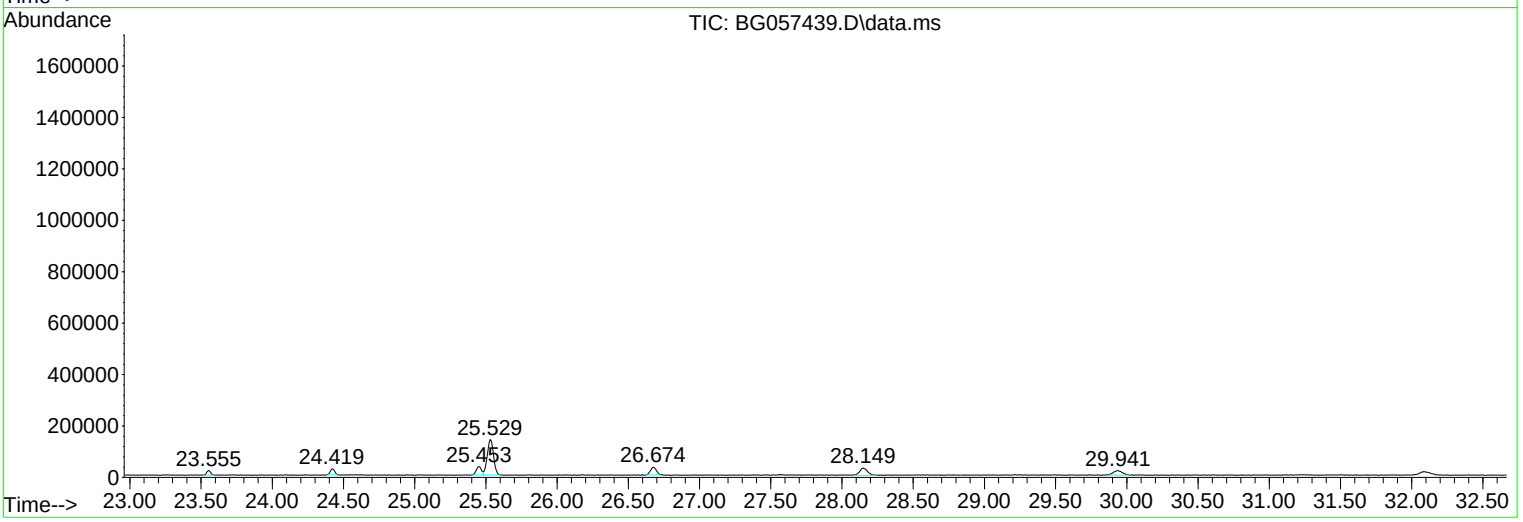
Instrument :
BNA_G
ClientSampleId :
PB152548BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P







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Data File : BG057439.D
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Instrument :
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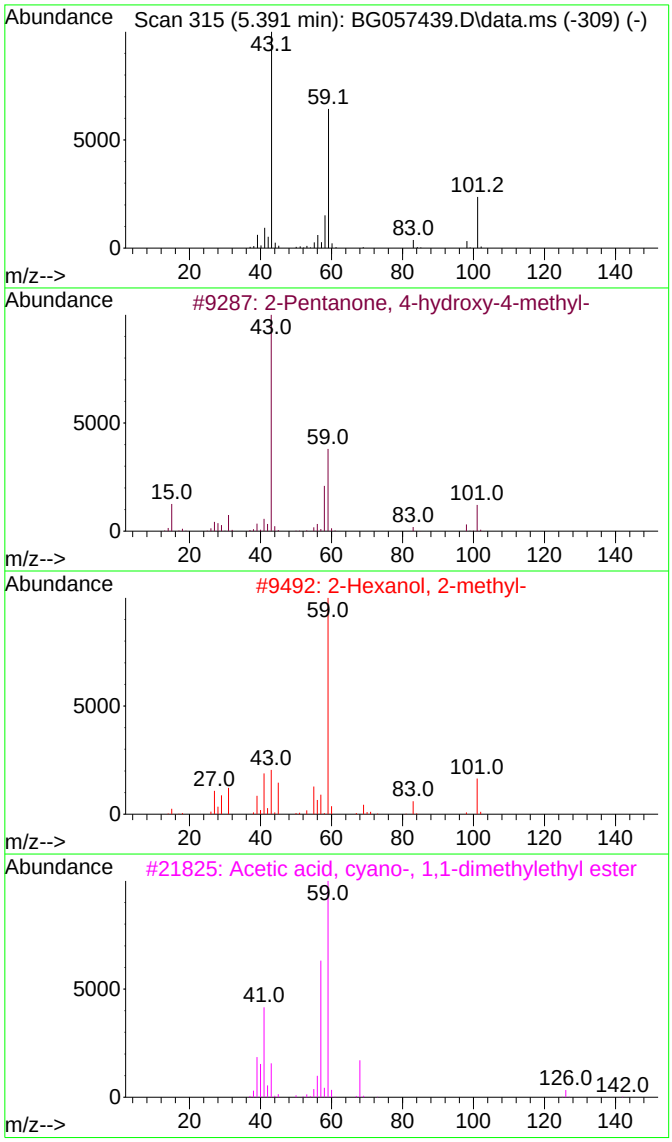
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

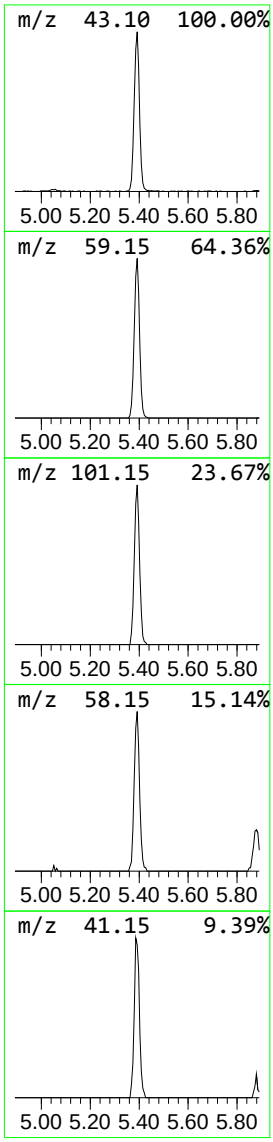
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.391	39.05 ng	225500	1,4-Dichlorobenzene-d4	8.358

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10





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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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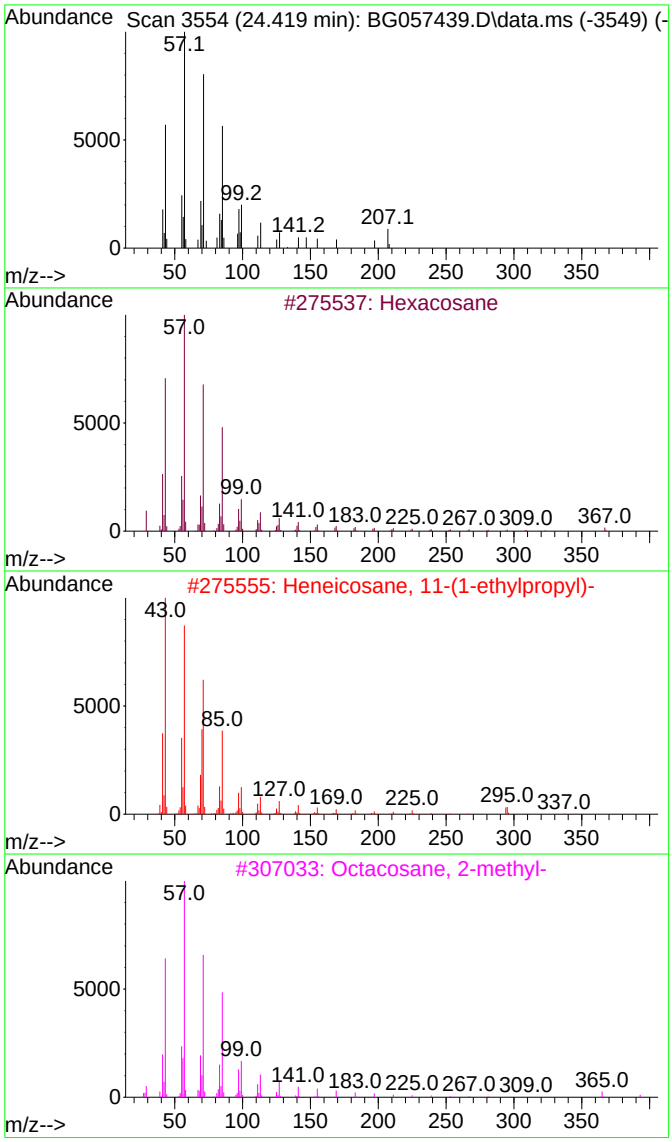
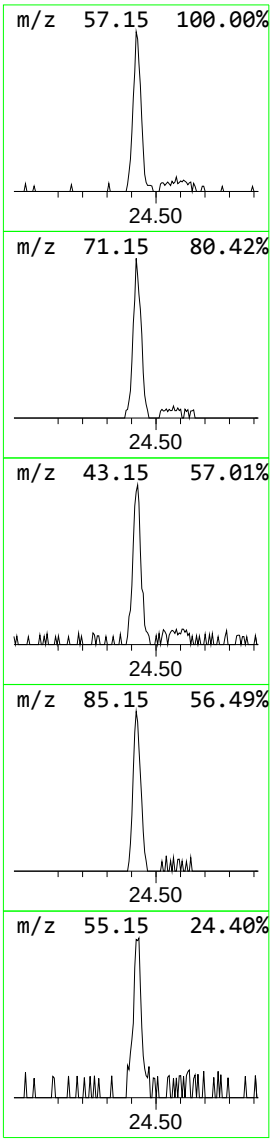
Peak Number 2 Hexacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.419	2.36 ng	49143	Perylene-d12	25.535

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	90
3	Octacosane, 2-methyl-	408	C29H60	001560-98-1	87
4	Heptadecane	240	C17H36	000629-78-7	86
5	Triacontane	422	C30H62	000638-68-6	86





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Data File : BG057439.D
Acq On : 16 May 2023 10:31
Operator : CG/JU
Sample : PB152548BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PB152548BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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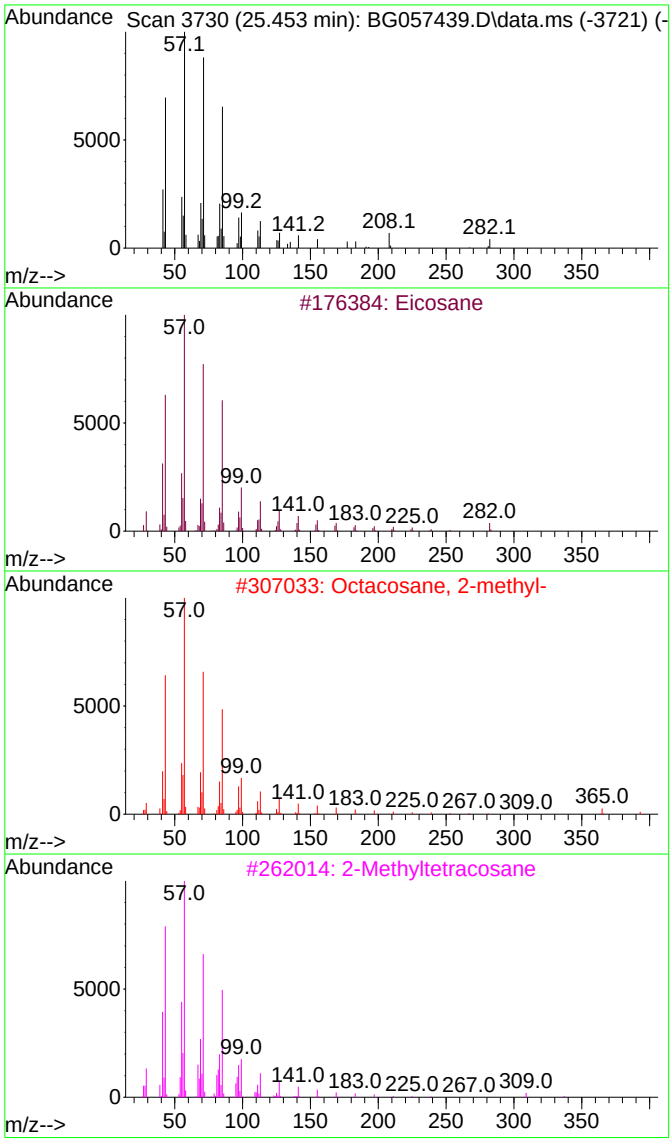
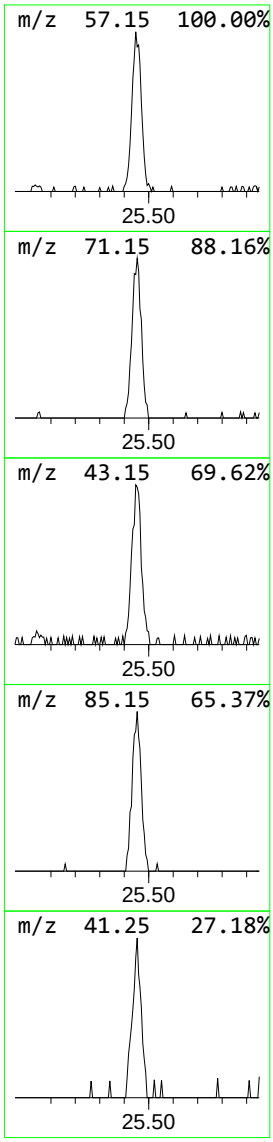
Peak Number 3 Eicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.453	4.21 ng	87510	Perylene-d12	25.535

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	96
2	Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
3	2-Methyltetracosane	352	C25H52	001560-78-7	91
4	Hexacosane	366	C26H54	000630-01-3	87
5	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	87





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Data File : BG057439.D
Acq On : 16 May 2023 10:31
Operator : CG/JU
Sample : PB152548BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PB152548BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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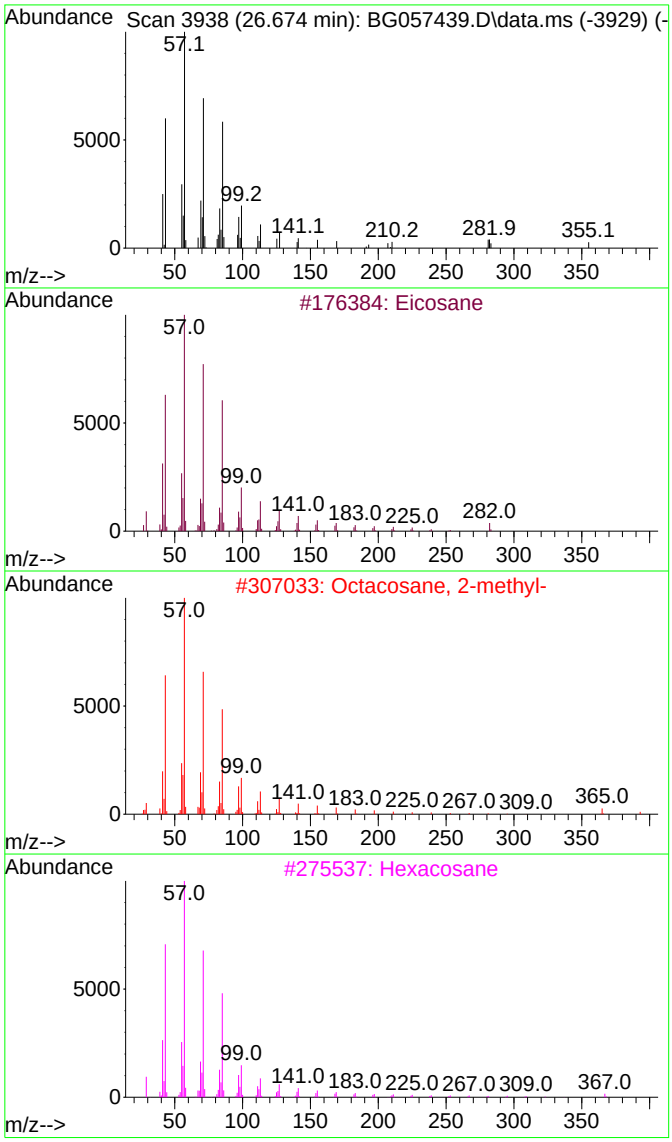
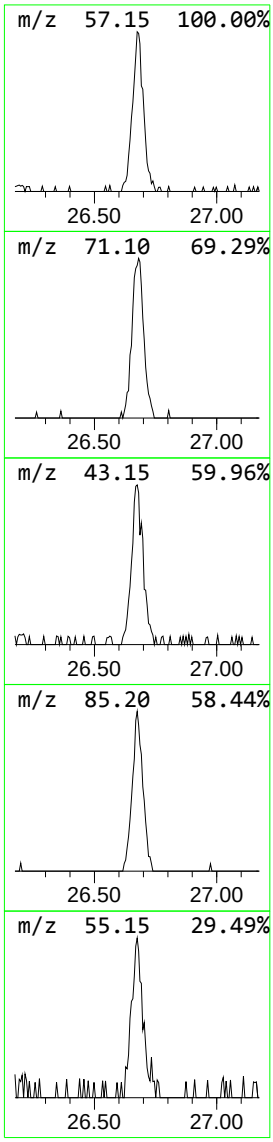
Peak Number 4 Octacosane, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.674	4.23 ng	87976	Perylene-d12	25.535

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	93
2	Octacosane, 2-methyl-	408	C29H60	001560-98-1	87
3	Hexacosane	366	C26H54	000630-01-3	87
4	Heneicosane	296	C21H44	000629-94-7	87
5	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	86





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051623\
Data File : BG057439.D
Acq On : 16 May 2023 10:31
Operator : CG/JU
Sample : PB152548BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PB152548BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042723.M
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TIC Library : C:\Database\NIST20.L
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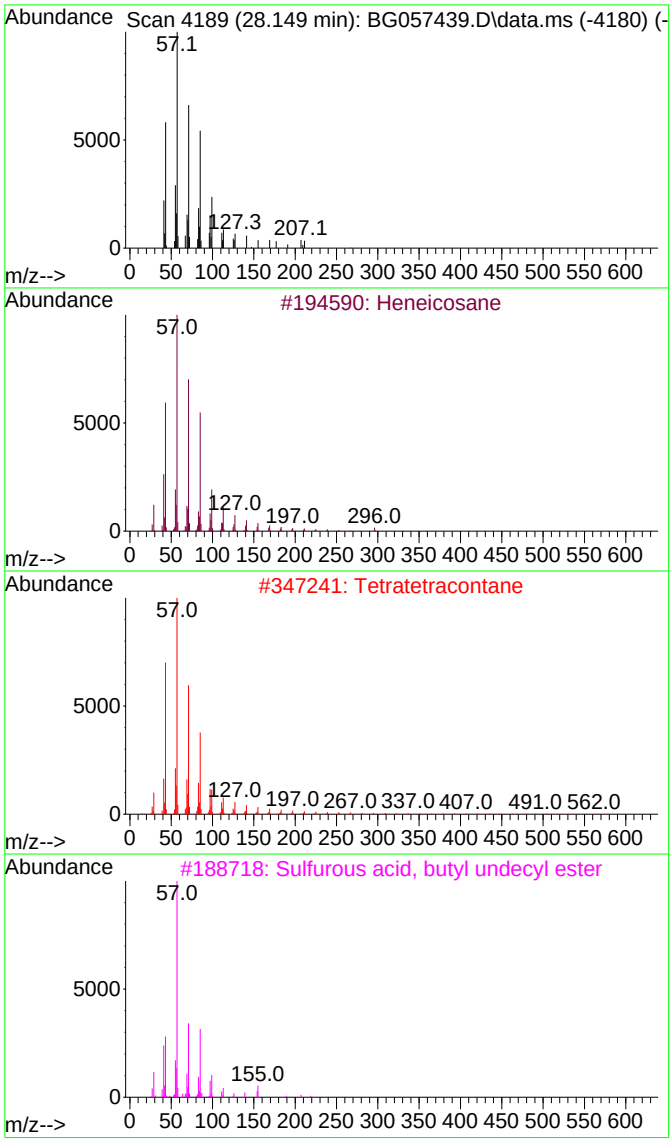
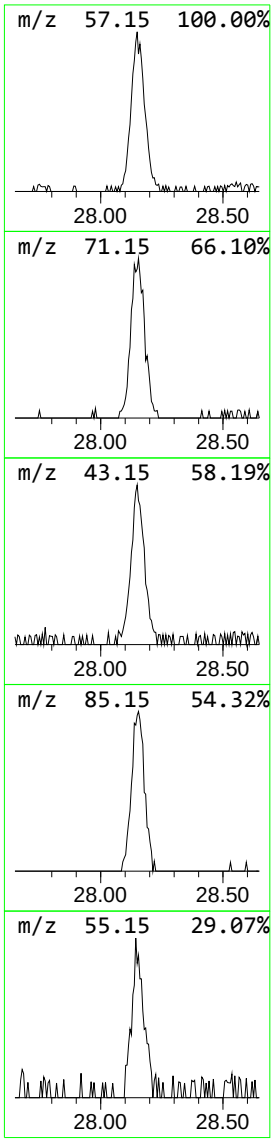
Peak Number 5 Heneicosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.149	5.15 ng	107004	Perylene-d12	25.535

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	87
2	Tetratetracontane	619	C44H90	007098-22-8	87
3	Sulfurous acid, butyl undecyl ester	292	C15H32O3S	1000309-17-8	86
4	Hexacosane	366	C26H54	000630-01-3	83
5	Pentacosane	352	C25H52	000629-99-2	83





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Operator : CG/JU
Sample : PB152548BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PB152548BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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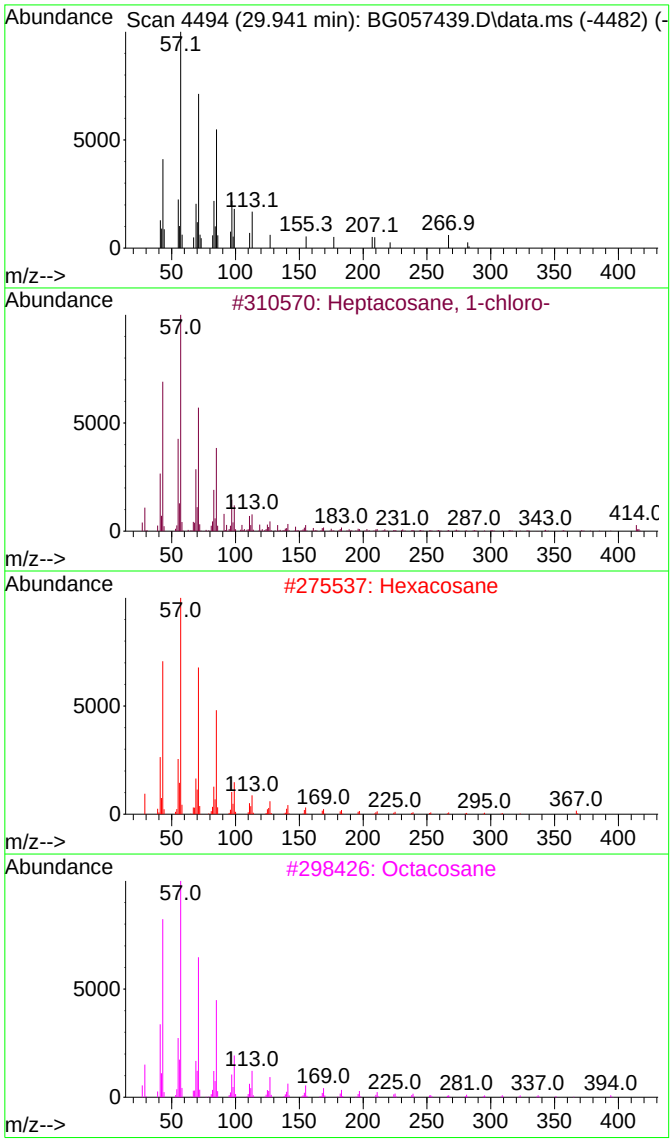
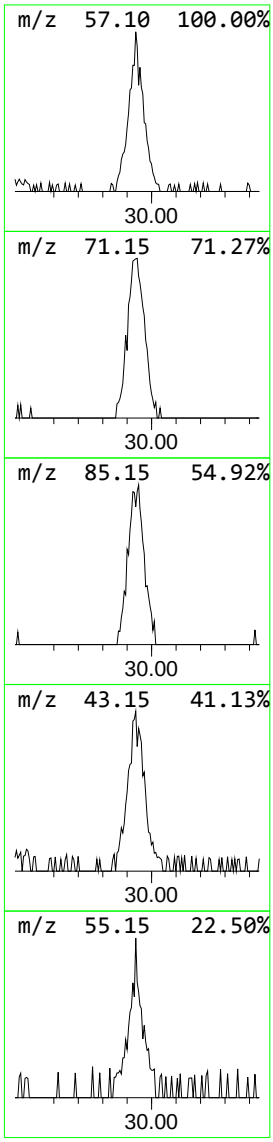
Peak Number 6 Heptacosane, 1-chloro- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
29.941	3.80 ng	79057	Perylene-d12	25.535

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	83
2	Hexacosane	366	C26H54	000630-01-3	80
3	Octacosane	394	C28H58	000630-02-4	80
4	Tritetracontane	605	C43H88	007098-21-7	78
5	Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	78





Tentatively Identified Compound (LSC) summary

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-...	5.391	39.0	ng	225500	1	8.358	115503	20.0
Hexacosane	24.419	2.4	ng	49143	6	25.535	415713	20.0
Eicosane	25.453	4.2	ng	87510	6	25.535	415713	20.0
Octacosane, 2-m...	26.674	4.2	ng	87976	6	25.535	415713	20.0
Heneicosane	28.149	5.2	ng	107004	6	25.535	415713	20.0
Heptacosane, 1-...	29.941	3.8	ng	79057	6	25.535	415713	20.0