LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040124\
Data File : BG060718.D
Acq On : 1 Apr 2024 16:46
Operator : MA/JU
Sample : PB159867BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PB159867BL

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-BG032924.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG060718.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.098	14	19	29	rVB3	43459	81372	1.04%	0.258%
2	5.079	350	356	364	rBV	85465	130724	1.67%	0.415%
3	5.537	427	434	446	rBV	1606907	2475112	31.68%	7.855%
4	7.111	692	702	715	rBV	1631895	2808944	35.95%	8.915%
5	7.958	839	846	853	rVB	291767	477416	6.11%	1.515%
6	9.109	1034	1042	1051	rBV	899281	1538399	19.69%	4.882%
7	10.754	1314	1322	1329	rBV	398314	698697	8.94%	2.217%
8	13.210	1732	1740	1748	rBV	2517315	3955390	50.62%	12.553%
9	14.585	1967	1974	1983	rVB	681179	1061836	13.59%	3.370%
10	16.072	2218	2227	2239	rBV	2095965	3191439	40.84%	10.129%
11	17.329	2434	2441	2448	rVB	1070704	1537122	19.67%	4.878%
12	19.679	2836	2841	2847	rBV	154473	178019	2.28%	0.565%
13	19.961	2882	2889	2901	rVB	5552363	7813573	100.00%	24.798%
14	20.725	3014	3019	3024	rBV	129042	151265	1.94%	0.480%
15	21.589	3159	3166	3175	rBV2	1106534	1788407	22.89%	5.676%
16	23.151	3426	3432	3440	rVB	80677	151844	1.94%	0.482%
17	23.956	3562	3569	3576	rBV	106555	231491	2.96%	0.735%
18	24.726	3689	3700	3712	rBV2	697379	1922724	24.61%	6.102%
19	24.908	3723	3731	3742	rVB2	130554	328353	4.20%	1.042%
20	26.042	3915	3924	3936	rBV3	110783	338149	4.33%	1.073%
21	27.399	4142	4155	4170	rBV3	98026	381791	4.89%	1.212%
22	29.045	4422	4435	4447	rBV4	59169	266419	3.41%	0.846%

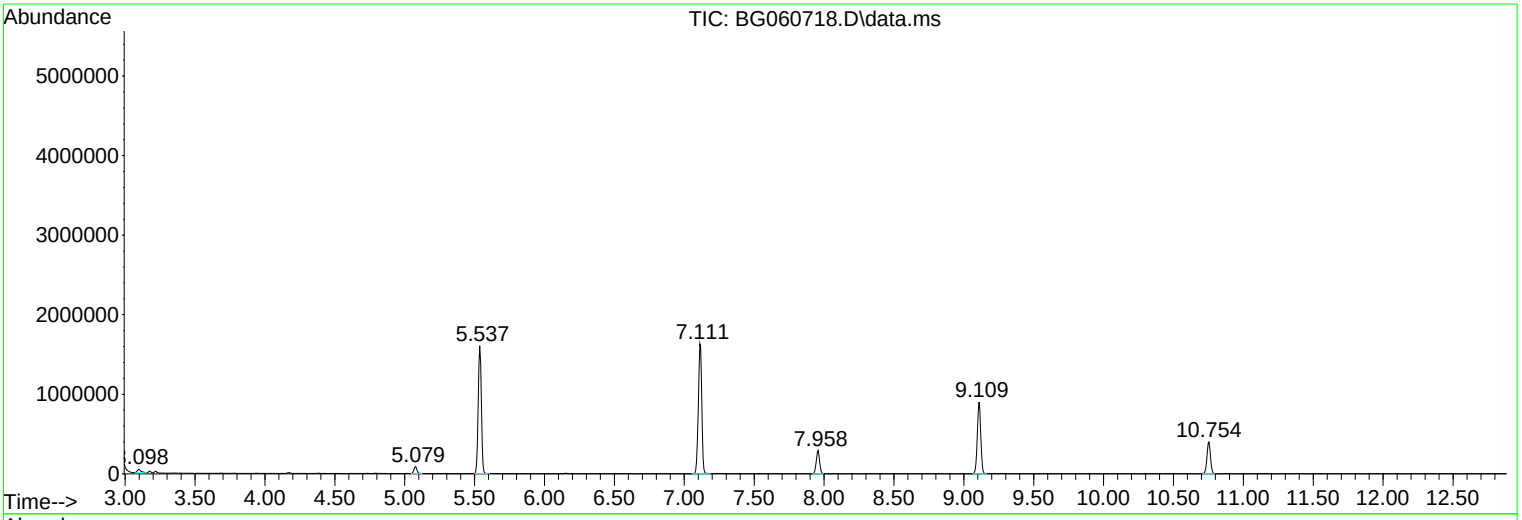
Sum of corrected areas: 31508486

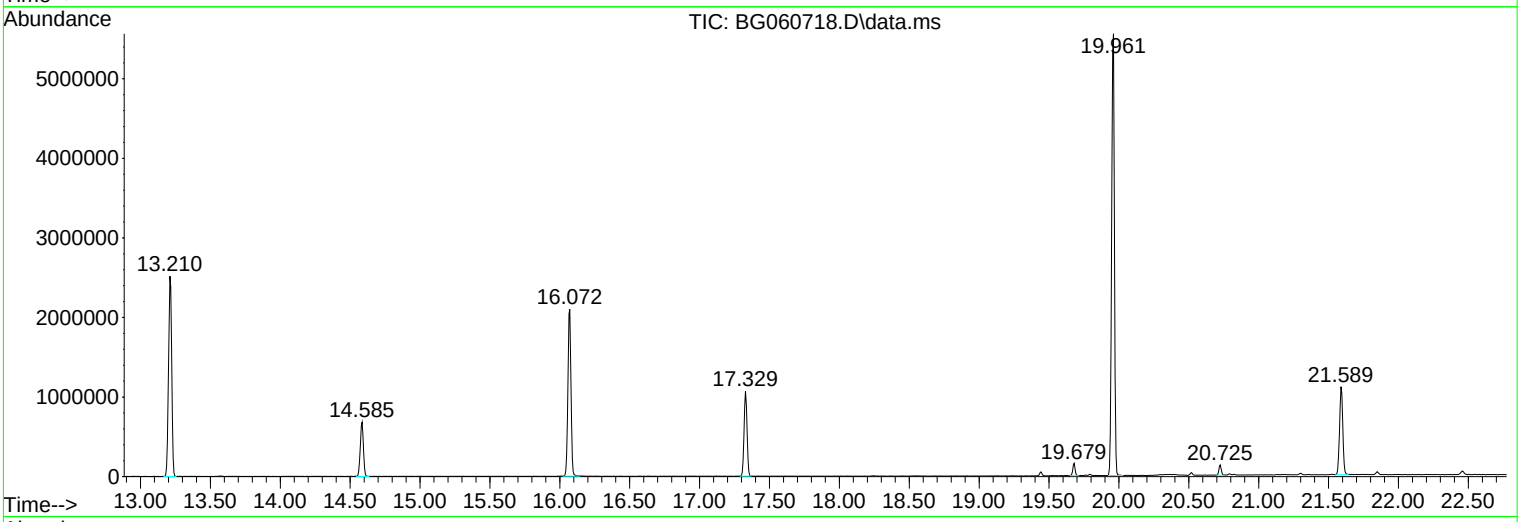
Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040124\
Data File : BG060718.D
Acq On : 1 Apr 2024 16:46
Operator : MA/JU
Sample : PB159867BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

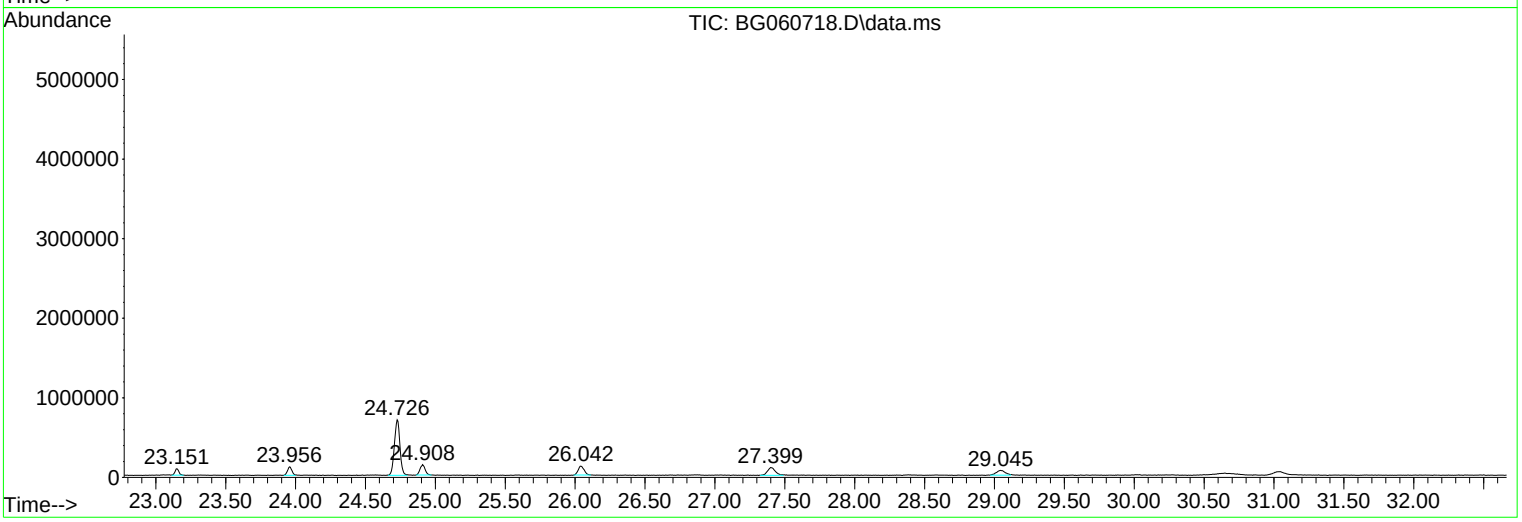
Instrument :
BNA_G
ClientSampleId :
PB159867BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG032924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040124\
Data File : BG060718.D
Acq On : 1 Apr 2024 16:46
Operator : MA/JU
Sample : PB159867BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PB159867BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG032924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

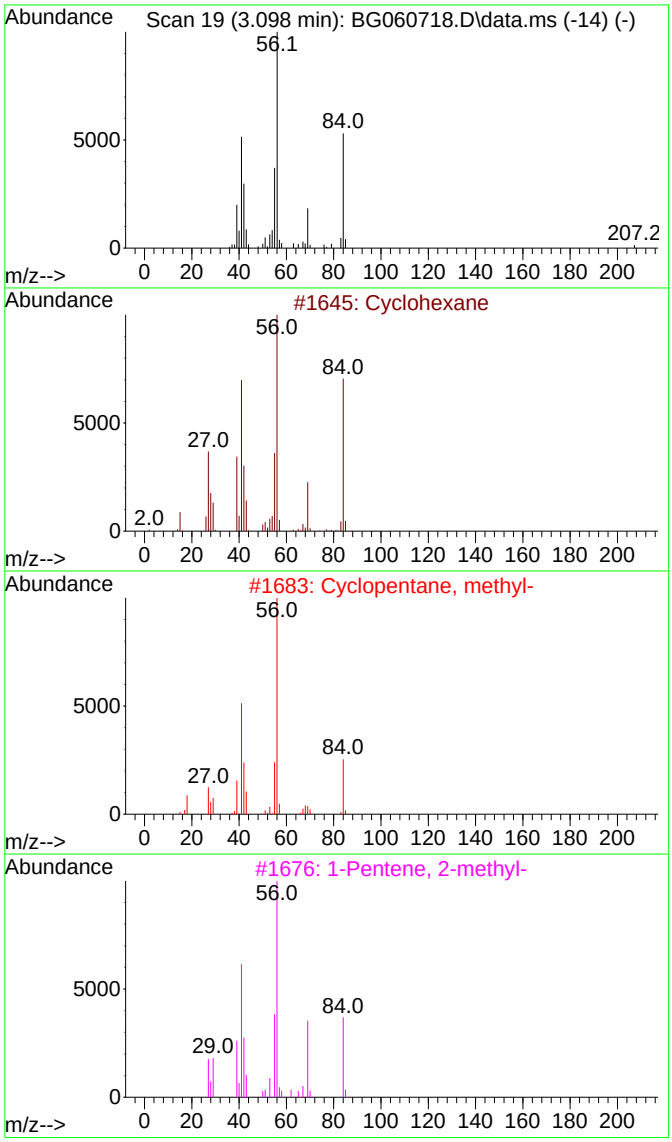
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

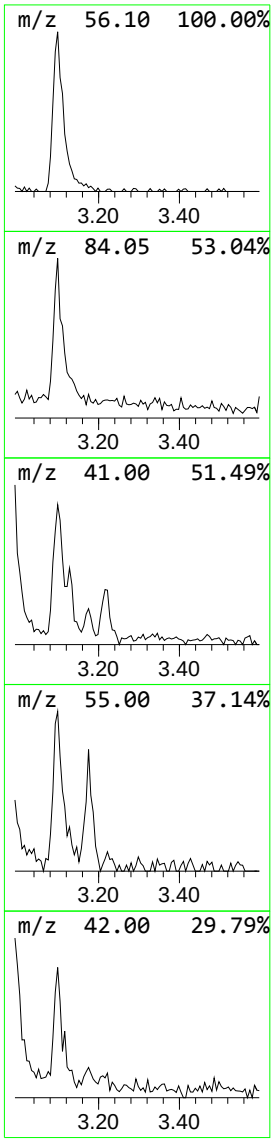
****

Peak Number 1 Cyclohexane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.098	3.41 ng	81372	1,4-Dichlorobenzene-d4	7.957

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane	84	C6H12	000110-82-7	91
2	Cyclopentane, methyl-	84	C6H12	000096-37-7	80
3	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	72
4	Cyclobutanone, 2-methyl-	84	C5H8O	001517-15-3	64
5	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040124\
Data File : BG060718.D
Acq On : 1 Apr 2024 16:46
Operator : MA/JU
Sample : PB159867BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PB159867BL

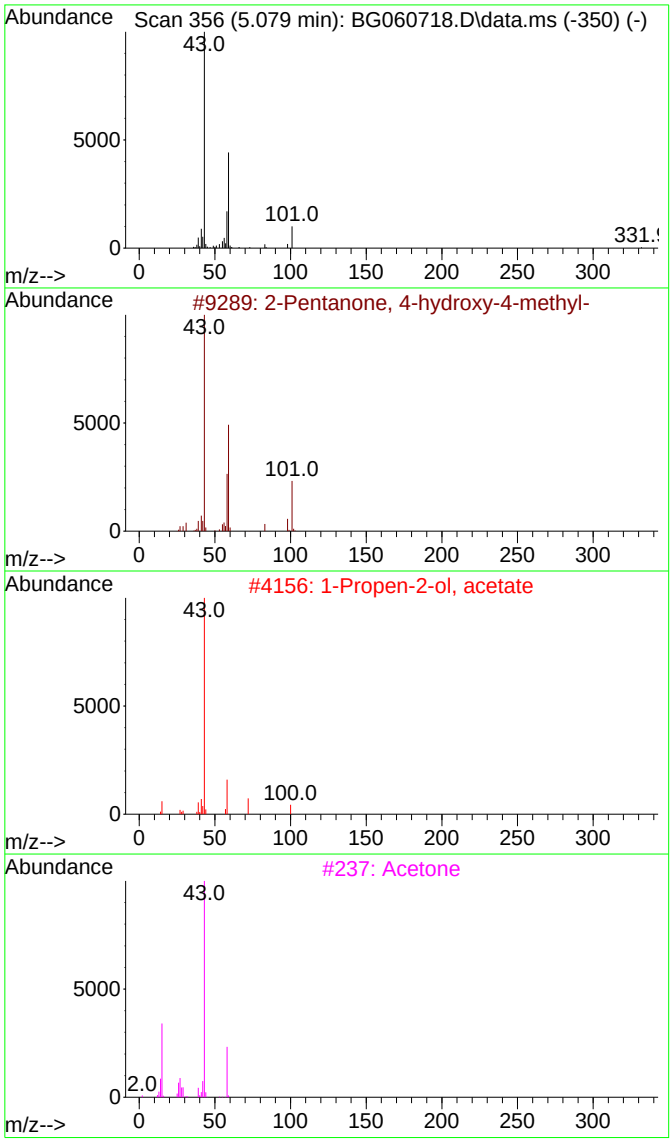
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG032924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

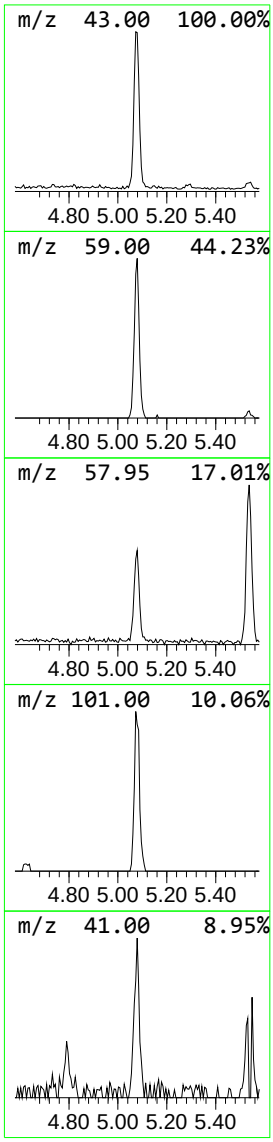
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.079	5.48 ng	130724	1,4-Dichlorobenzene-d4	7.957

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	78
2	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
3	Acetone	58	C3H6O	000067-64-1	10
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	5-Oxohexanenitrile	111	C6H9NO	010412-98-3	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040124\
Data File : BG060718.D
Acq On : 1 Apr 2024 16:46
Operator : MA/JU
Sample : PB159867BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PB159867BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG032924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

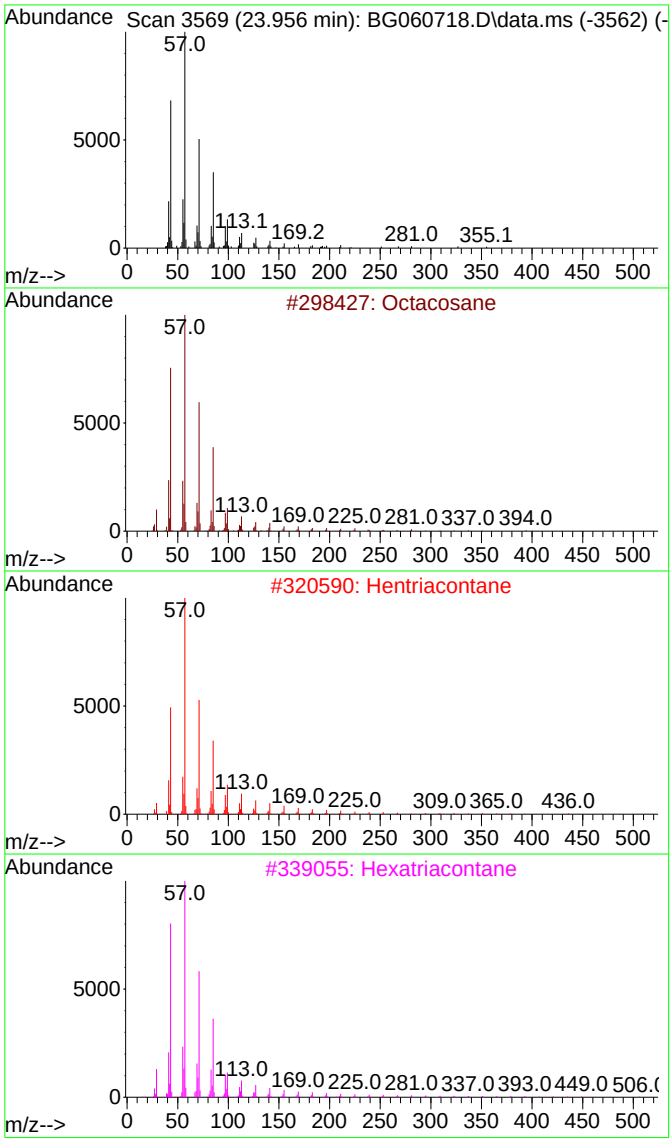
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

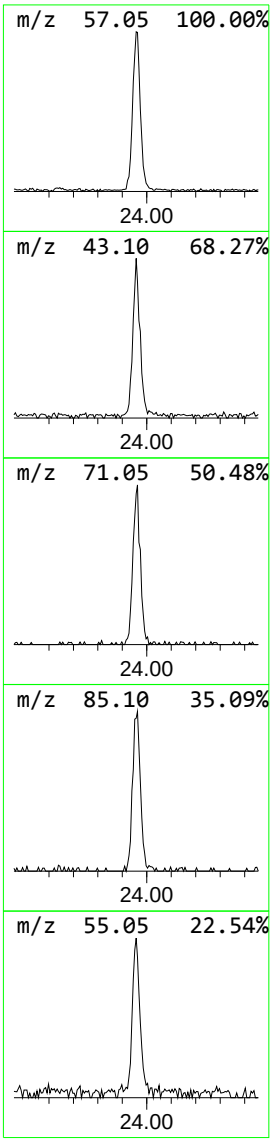
****

Peak Number 3 Octacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.956	2.41 ng	231491	Perylene-d12	24.726

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Hentriacontane	437	C31H64	000630-04-6	91
3	Hexatriacontane	507	C36H74	000630-06-8	91
4	Octacosane, 2-methyl-	408	C29H60	001560-98-1	90
5	Heneicosane	296	C21H44	000629-94-7	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040124\
Data File : BG060718.D
Acq On : 1 Apr 2024 16:46
Operator : MA/JU
Sample : PB159867BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PB159867BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG032924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

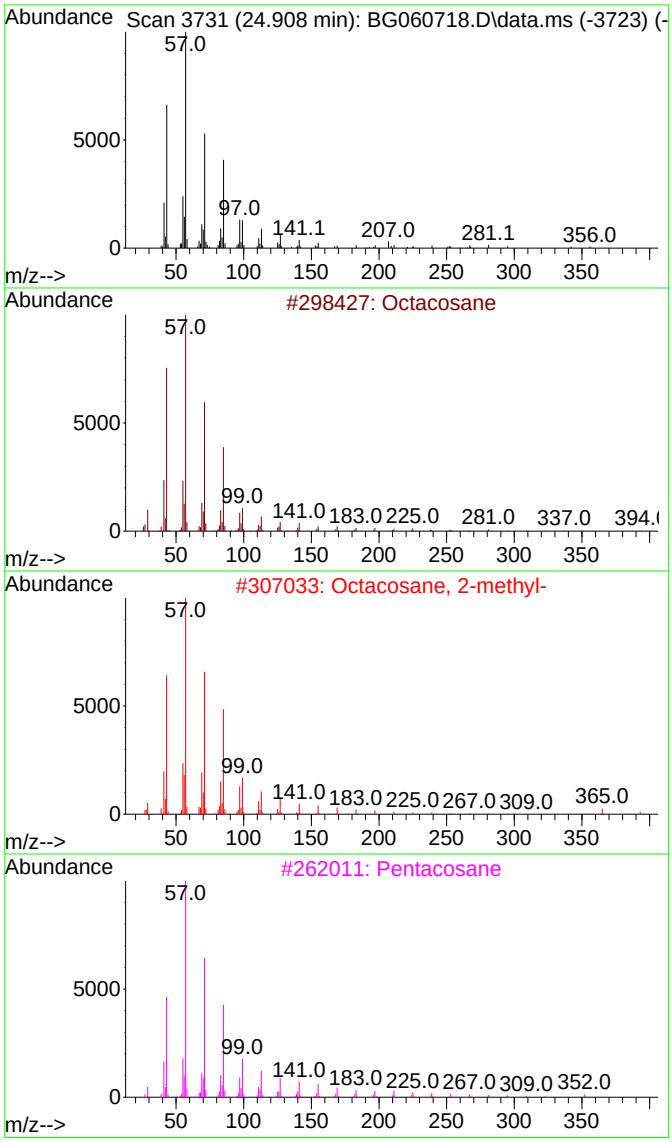
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

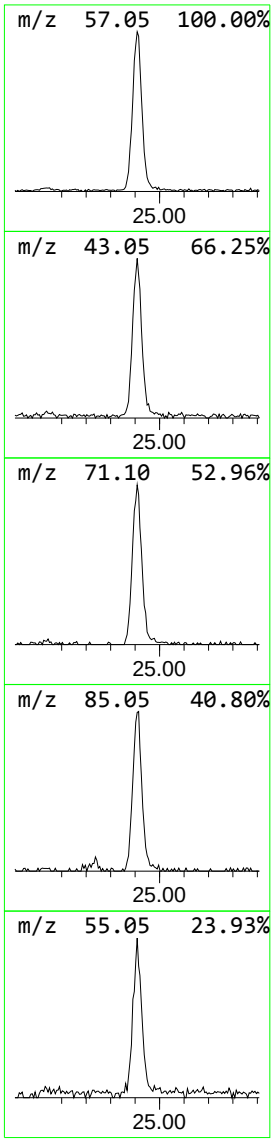
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.908	3.42 ng	328353	Perylene-d12	24.726

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Octacosane, 2-methyl-	408	C29H60	001560-98-1	90
3	Pentacosane	352	C25H52	000629-99-2	90
4	Pentadecane	212	C15H32	000629-62-9	87
5	Heneicosane	296	C21H44	000629-94-7	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040124\
Data File : BG060718.D
Acq On : 1 Apr 2024 16:46
Operator : MA/JU
Sample : PB159867BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PB159867BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG032924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

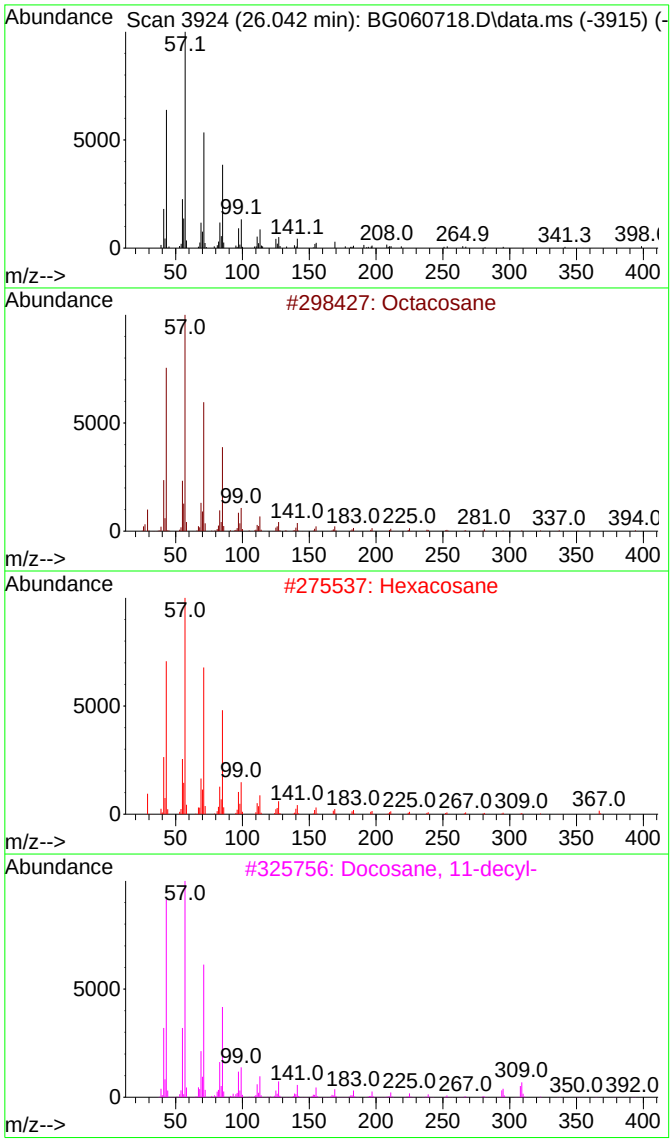
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

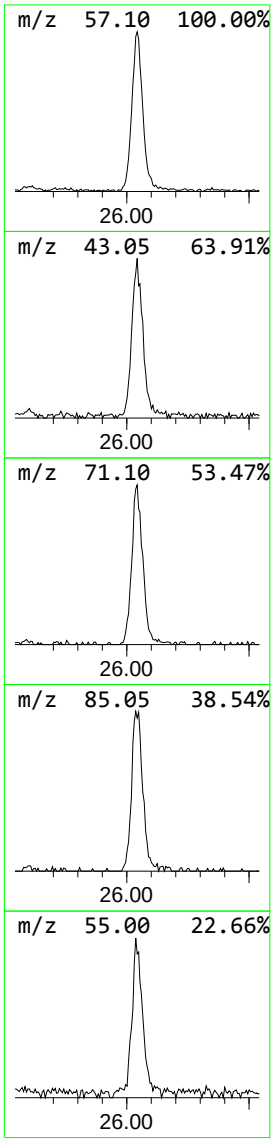
****

Peak Number 5 Hexacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.042	3.52 ng	338149	Perylene-d12	24.726

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	90
2	Hexacosane	366	C26H54	000630-01-3	87
3	Docosane, 11-decyl-	451	C32H66	055401-55-3	87
4	Tetratetracontane	619	C44H90	007098-22-8	87
5	Heneicosane, 11-decyl-	437	C31H64	055320-06-4	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040124\
Data File : BG060718.D
Acq On : 1 Apr 2024 16:46
Operator : MA/JU
Sample : PB159867BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PB159867BL

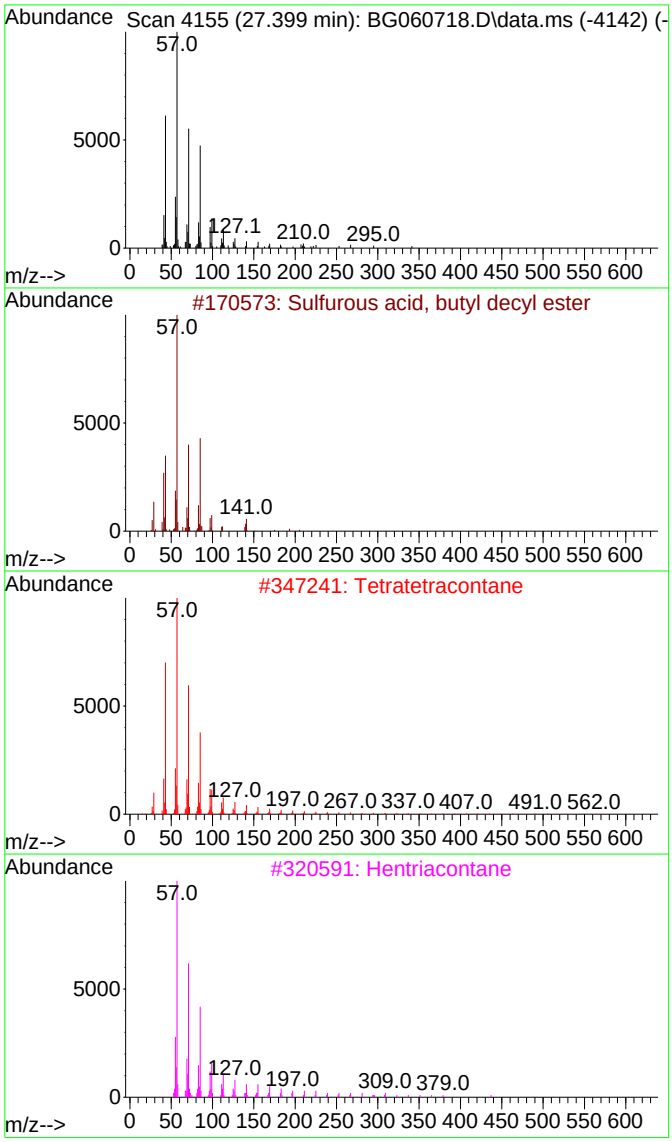
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG032924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

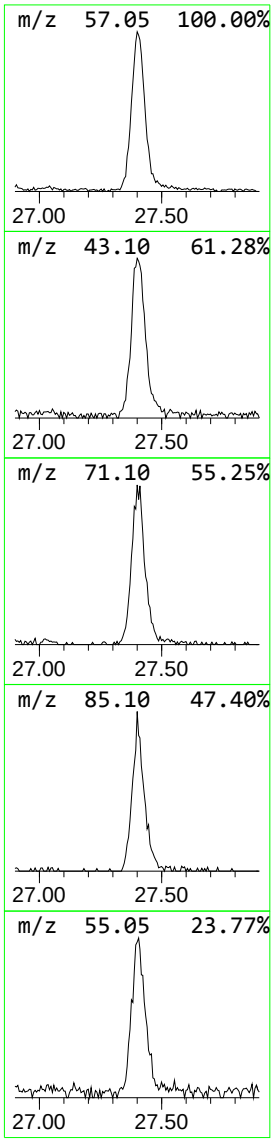
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Sulfurous acid, butyl decyl... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.399	3.97 ng	381791	Perylene-d12	24.726

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, butyl decyl ester	278	C14H30O3S	1000309-17-7	80
2	Tetratetracontane	619	C44H90	007098-22-8	68
3	Hentriacontane	437	C31H64	000630-04-6	68
4	Heneicosane, 11-decyl-	437	C31H64	055320-06-4	64
5	Sulfurous acid, butyl undecyl ester	292	C15H32O3S	1000309-17-8	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040124\
Data File : BG060718.D
Acq On : 1 Apr 2024 16:46
Operator : MA/JU
Sample : PB159867BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PB159867BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG032924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

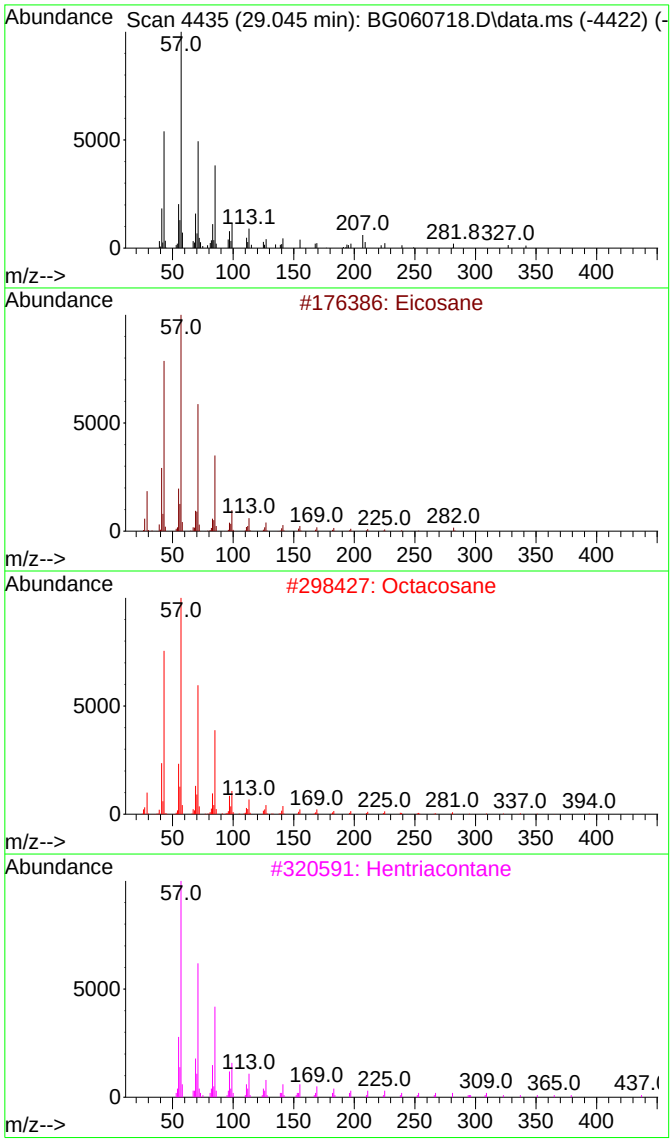
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

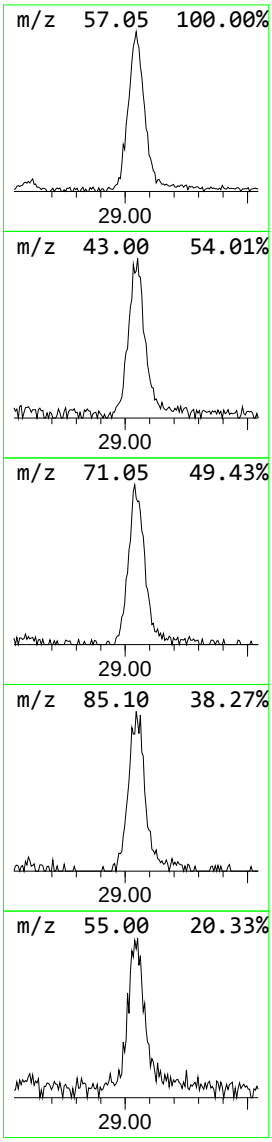
****

Peak Number 7 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
29.045	2.77 ng	266419	Perylene-d12	24.726

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	93
2	Octacosane	394	C28H58	000630-02-4	87
3	Hentriacontane	437	C31H64	000630-04-6	83
4	Docosane	310	C22H46	000629-97-0	83
5	Tetracosane	338	C24H50	000646-31-1	83





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040124\
Data File : BG060718.D
Acq On : 1 Apr 2024 16:46
Operator : MA/JU
Sample : PB159867BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PB159867BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG032924.M
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
Cyclohexane	3.098	3.4	ng	81372	1	7.957	477416	20.0
2-Pentanone, 4-...	5.079	5.5	ng	130724	1	7.957	477416	20.0
Octacosane	23.956	2.4	ng	231491	6	24.726	1922720	20.0
Octacosane, 2-m...	24.908	3.4	ng	328353	6	24.726	1922720	20.0
Hexacosane	26.042	3.5	ng	338149	6	24.726	1922720	20.0
Sulfurous acid,...	27.399	4.0	ng	381791	6	24.726	1922720	20.0
Eicosane	29.045	2.8	ng	266419	6	24.726	1922720	20.0