LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040824\
Data File : BG060831.D
Acq On : 8 Apr 2024 18:34
Operator : MA/JU
Sample : PB160000BL
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PB160000BL

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: BG060831.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.089	11	17	26	rVB4	28579	70050	1.07%	0.259%
2	5.069	348	354	362	rVB	70681	102470	1.57%	0.379%
3	5.534	426	433	447	rBV	1312770	1987873	30.38%	7.359%
4	7.114	692	702	714	rBV	1313004	2195946	33.56%	8.129%
5	7.948	836	844	851	rBV	233170	395528	6.04%	1.464%
6	9.100	1031	1040	1050	rBV	786329	1356727	20.73%	5.023%
7	10.745	1311	1320	1327	rBV	302791	540039	8.25%	1.999%
8	13.201	1731	1738	1749	rBV	2050354	3222378	49.25%	11.929%
9	14.576	1965	1972	1979	rBV	562909	866095	13.24%	3.206%
10	16.062	2217	2225	2235	rBV	2006632	3043908	46.52%	11.268%
11	17.326	2433	2440	2449	rBV	835746	1281232	19.58%	4.743%
12	19.664	2833	2838	2845	rVB	124166	141933	2.17%	0.525%
13	19.952	2880	2887	2892	rBV	4841389	6543523	100.00%	24.224%
14	20.704	3011	3015	3021	rVB	112945	121821	1.86%	0.451%
15	21.585	3158	3165	3174	rBV2	949119	1531753	23.41%	5.670%
16	22.425	3302	3308	3314	rBV2	41679	69765	1.07%	0.258%
17	23.113	3419	3425	3431	rBV	79200	138182	2.11%	0.512%
18	23.906	3554	3560	3570	rVB2	104945	233375	3.57%	0.864%
19	24.717	3687	3698	3708	rBV	583452	1616402	24.70%	5.984%
20	24.852	3712	3721	3732	rVB	129934	330696	5.05%	1.224%
21	25.968	3902	3911	3920	rBV4	110157	322533	4.93%	1.194%
22	27.308	4126	4139	4153	rBV3	100376	384535	5.88%	1.424%
23	28.941	4404	4417	4430	rVB5	63676	281928	4.31%	1.044%
24	30.898	4736	4750	4765	rVB6	45681	234063	3.58%	0.866%

Sum of corrected areas: 27012755

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040824\
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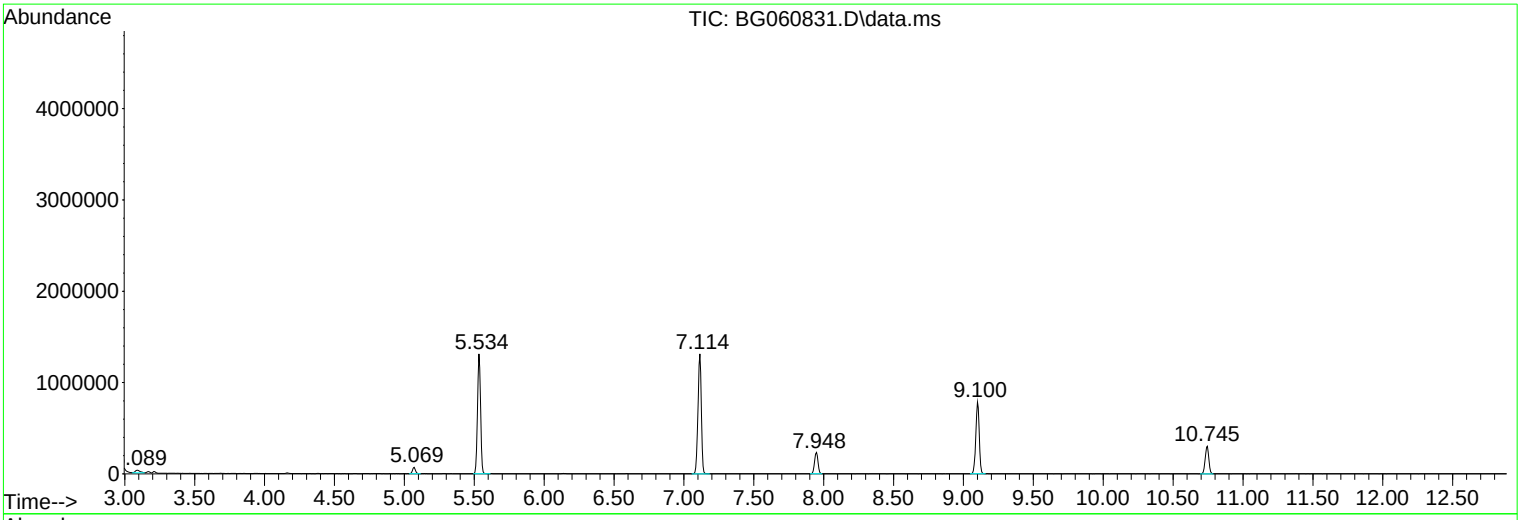
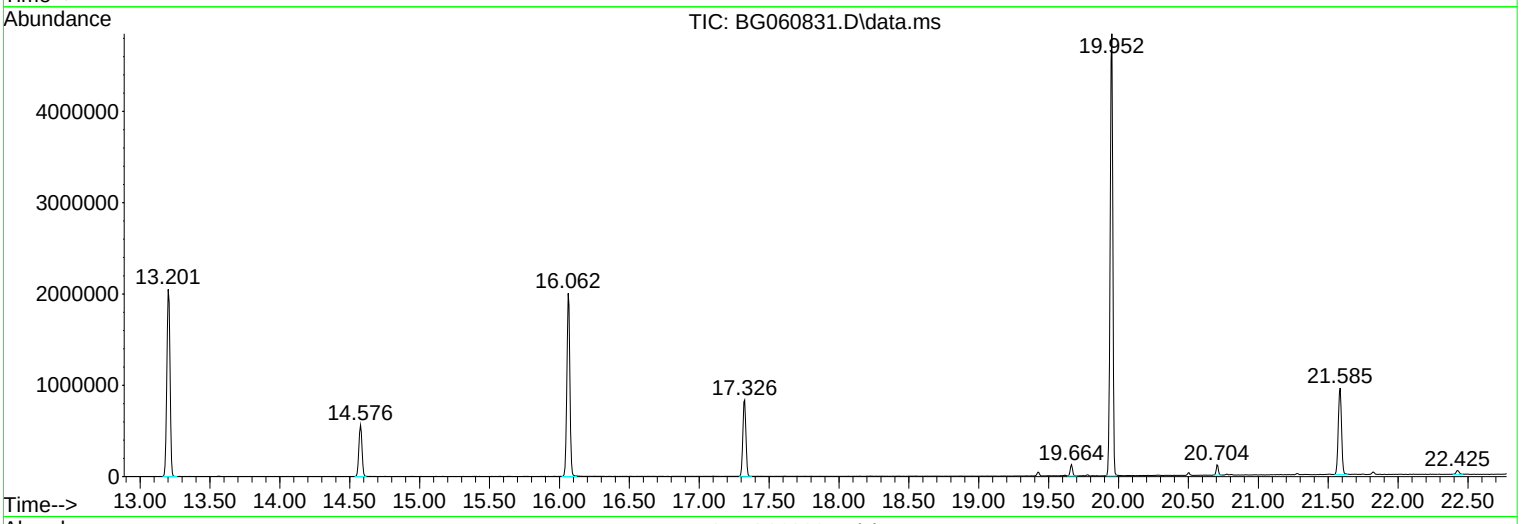
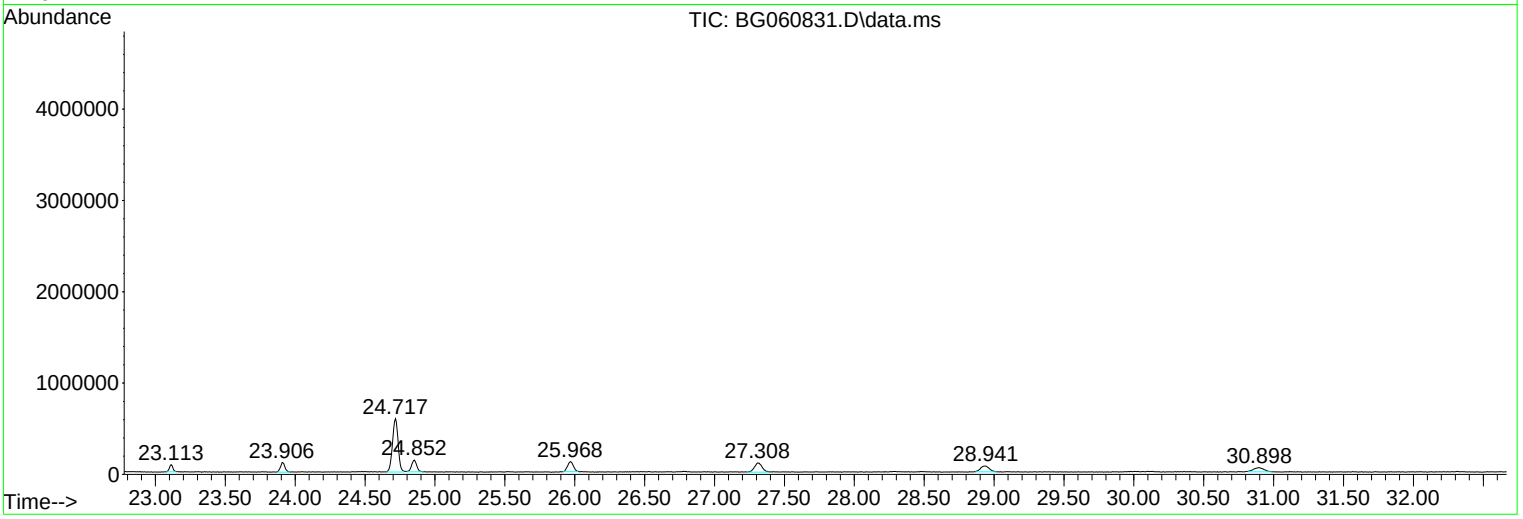
Instrument :
BNA_G
ClientSampleId :
PB160000BL

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







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Data File : BG060831.D
Acq On : 8 Apr 2024 18:34
Operator : MA/JU
Sample : PB160000BL
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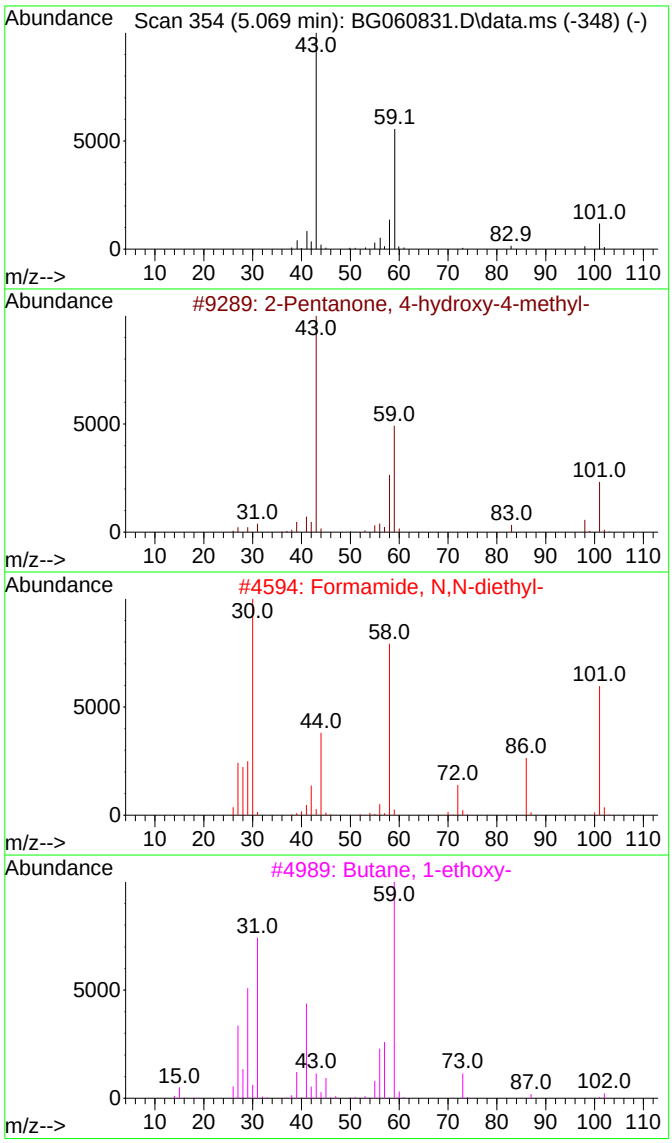
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

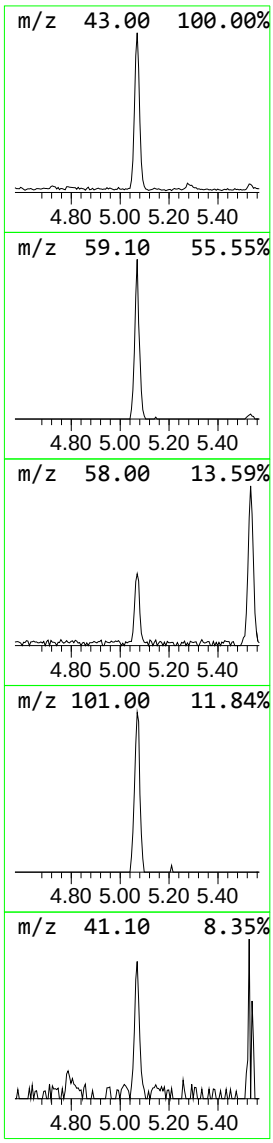
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.069	5.18 ng	102470	1,4-Dichlorobenzene-d4	7.948

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Formamide, N,N-diethyl-	101	C5H11NO	000617-84-5	9
3	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040824\
Data File : BG060831.D
Acq On : 8 Apr 2024 18:34
Operator : MA/JU
Sample : PB160000BL
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PB160000BL

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

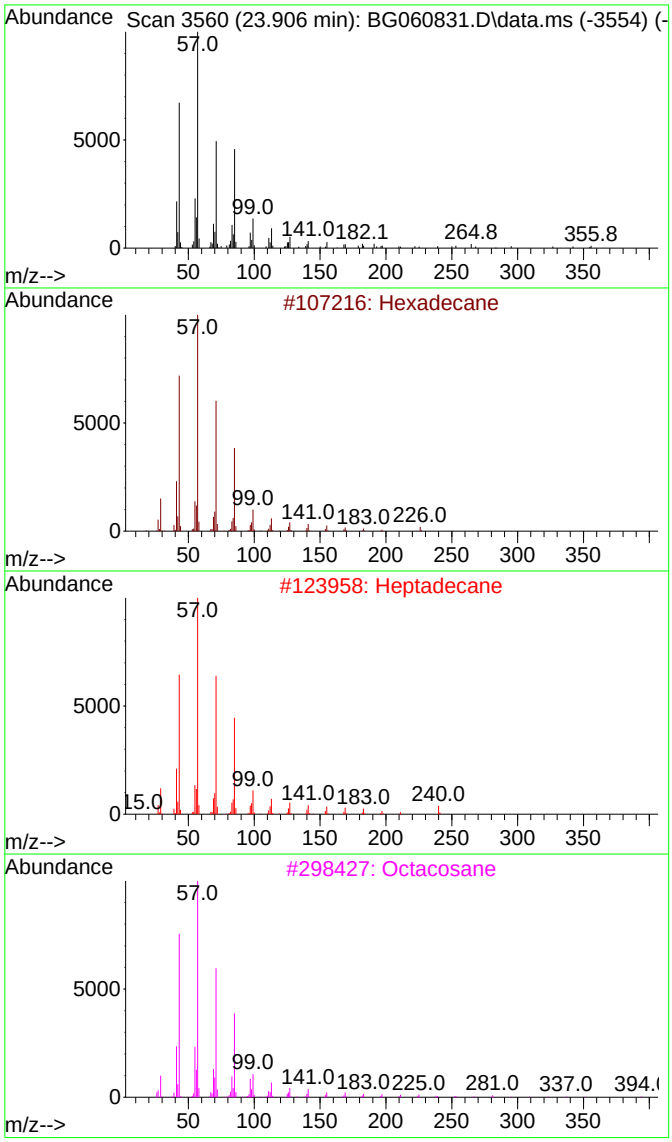
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

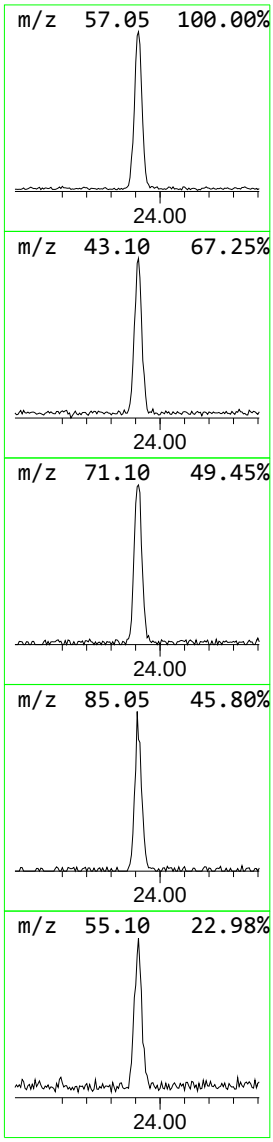
****

Peak Number 3 Hexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.906	2.89 ng	233375	Perylene-d12	24.717

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	87
2	Heptadecane	240	C17H36	000629-78-7	86
3	Octacosane	394	C28H58	000630-02-4	86
4	7-Methyl-octadecane	268	C19H40	1000192-63-3	76
5	Hexatriacontane	507	C36H74	000630-06-8	74





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040824\
Data File : BG060831.D
Acq On : 8 Apr 2024 18:34
Operator : MA/JU
Sample : PB160000BL
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PB160000BL

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

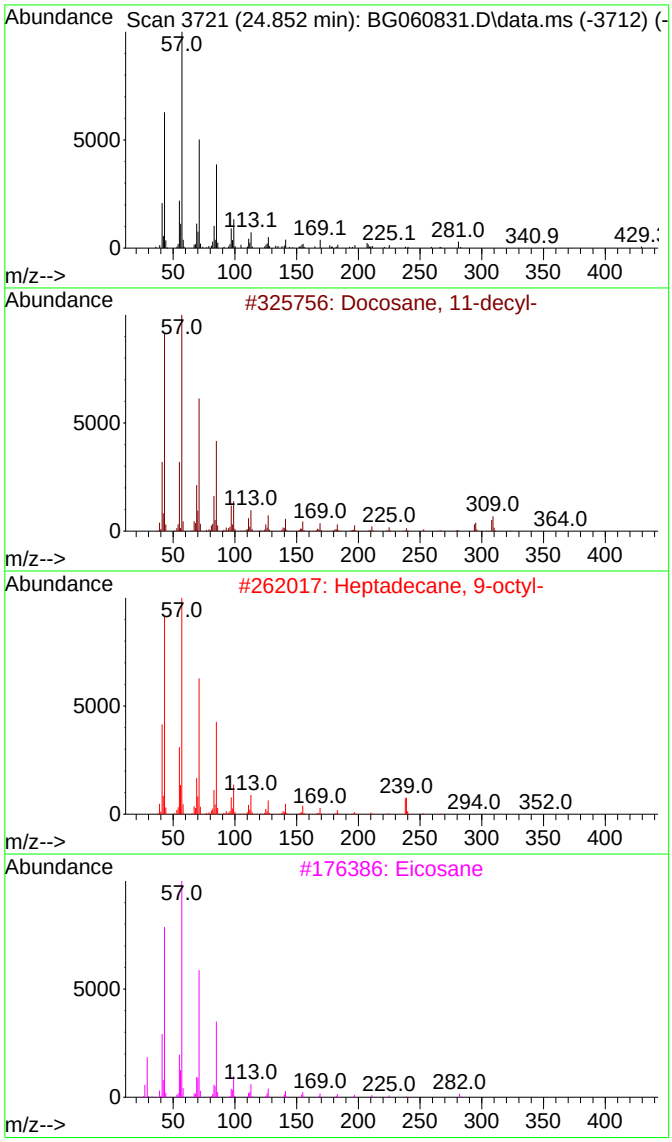
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

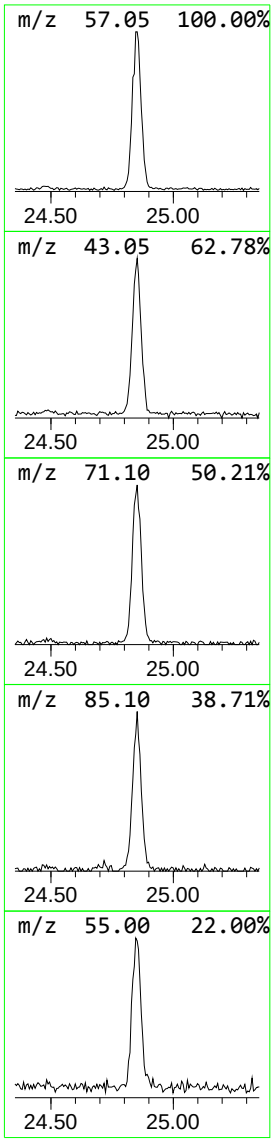
****

Peak Number 4 Docosane, 11-decyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.852	4.09 ng	330696	Perylene-d12	24.717

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosane, 11-decyl-	451	C32H66	055401-55-3	90
2	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90
3	Eicosane	282	C20H42	000112-95-8	83
4	Octacosane, 1-iodo-	520	C28H57I	1000406-32-2	83
5	Heneicosane	296	C21H44	000629-94-7	81





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040824\
Data File : BG060831.D
Acq On : 8 Apr 2024 18:34
Operator : MA/JU
Sample : PB160000BL
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PB160000BL

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

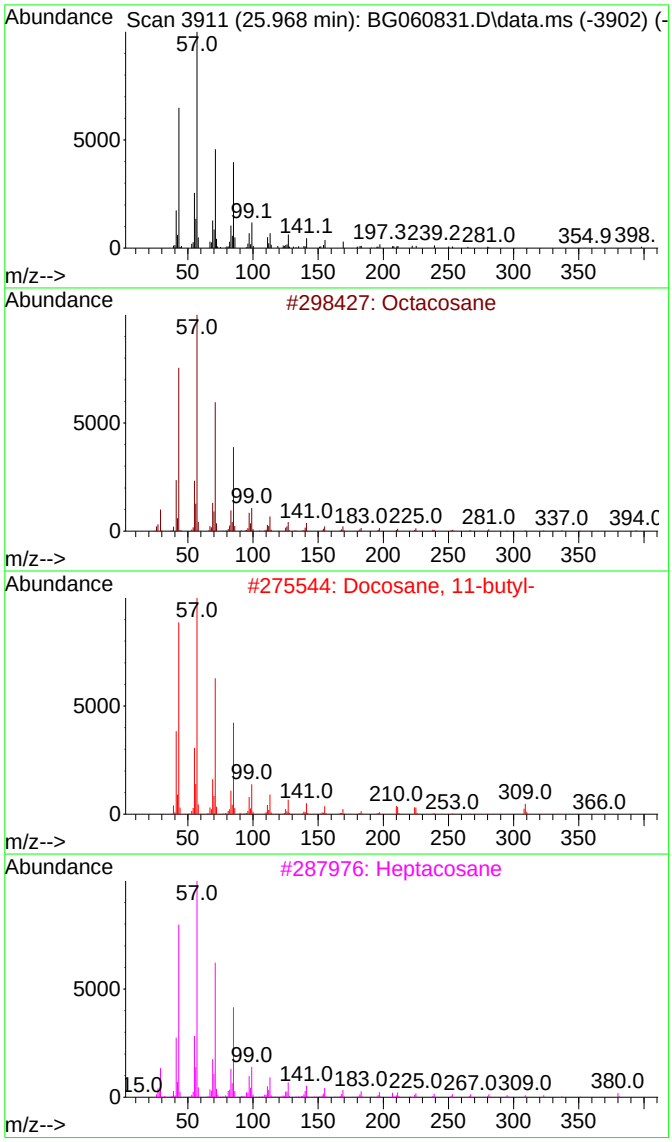
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

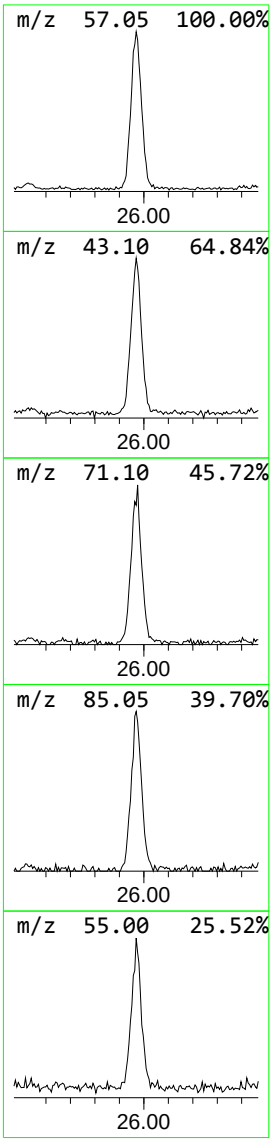
****

Peak Number 5 Octacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.968	3.99 ng	322533	Perylene-d12	24.717

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Docosane, 11-butyl-	366	C26H54	013475-76-8	91
3	Heptacosane	380	C27H56	000593-49-7	91
4	Heneicosane	296	C21H44	000629-94-7	87
5	Hexacosane	366	C26H54	000630-01-3	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040824\
Data File : BG060831.D
Acq On : 8 Apr 2024 18:34
Operator : MA/JU
Sample : PB160000BL
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PB160000BL

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
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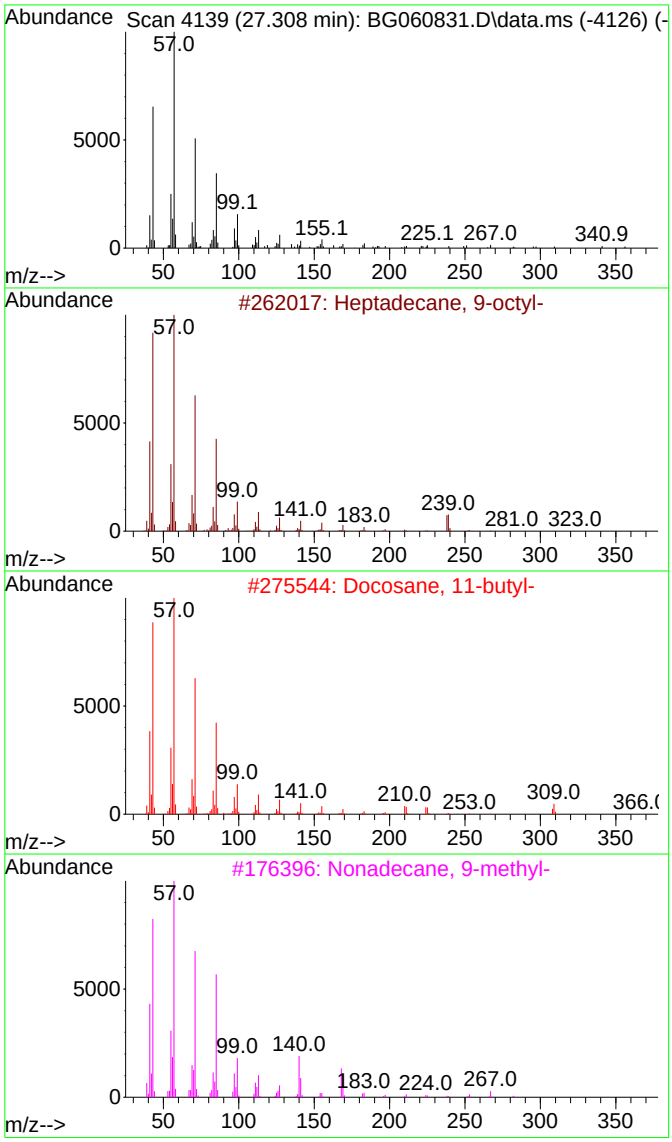
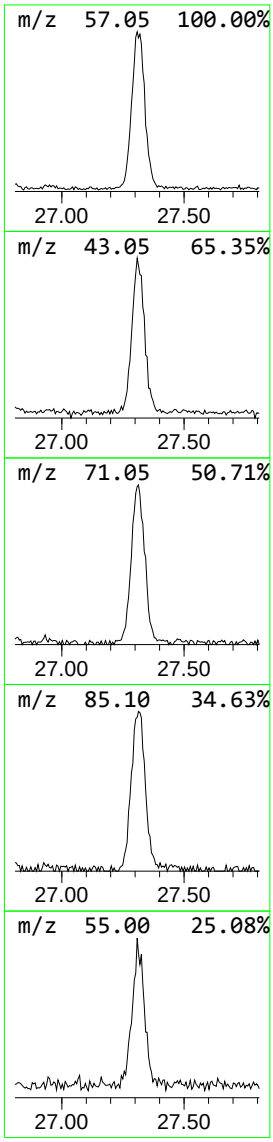
****

Peak Number 6 Heptadecane, 9-octyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.308	4.76 ng	384535	Perylene-d12	24.717

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
2	Docosane, 11-butyl-	366	C26H54	013475-76-8	91
3	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	90
4	Heneicosane	296	C21H44	000629-94-7	90
5	Eicosane	282	C20H42	000112-95-8	90





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Data File : BG060831.D
Acq On : 8 Apr 2024 18:34
Operator : MA/JU
Sample : PB160000BL
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PB160000BL

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

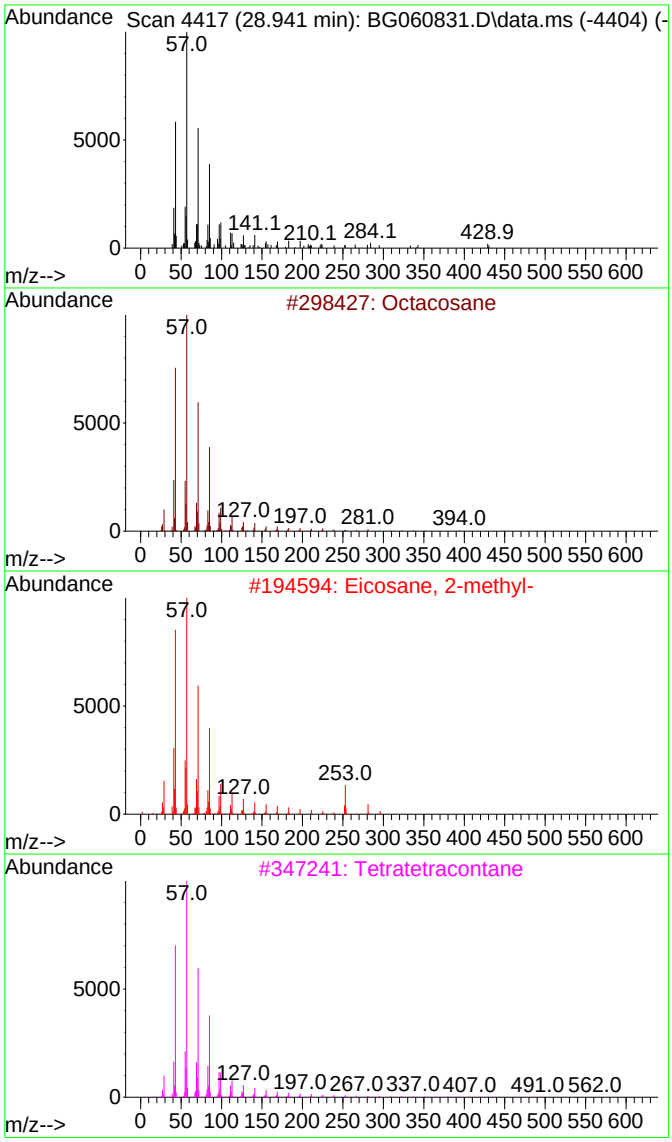
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

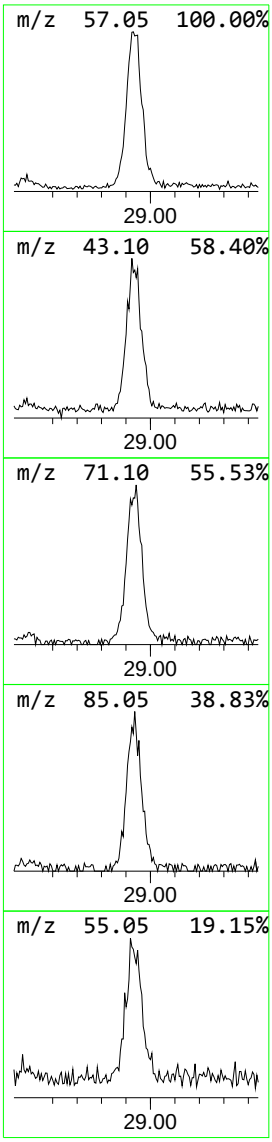
****

Peak Number 7 Eicosane, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.941	3.49 ng	281928	Perylene-d12	24.717

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	90
2	Eicosane, 2-methyl-	296	C21H44	001560-84-5	86
3	Tetratetracontane	619	C44H90	007098-22-8	86
4	Heptacosane	380	C27H56	000593-49-7	86
5	Heneicosane	296	C21H44	000629-94-7	80





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Operator : MA/JU
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Misc :
ALS Vial : 13 Sample Multiplier: 1

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

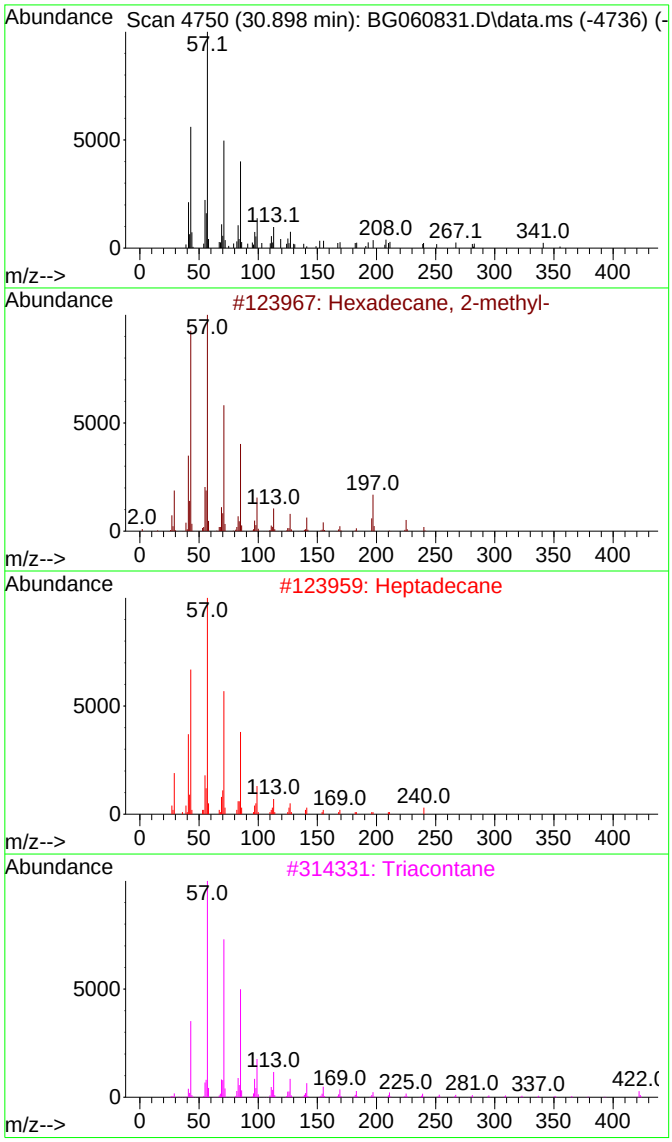
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

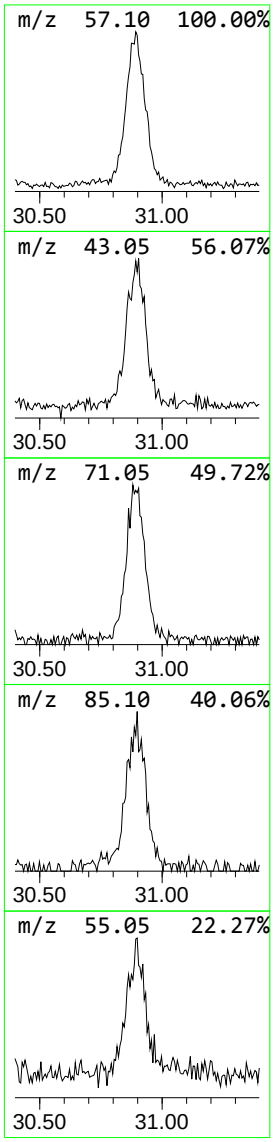
****

Peak Number 8 Hexadecane, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
30.898	2.90 ng	234063	Perylene-d12	24.717

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane, 2-methyl-	240	C17H36	001560-92-5	93
2	Heptadecane	240	C17H36	000629-78-7	90
3	Triacontane	422	C30H62	000638-68-6	83
4	Docosane	310	C22H46	000629-97-0	83
5	1-Iodoundecane	282	C11H23I	004282-44-4	83





Tentatively Identified Compound (LSC) summary

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Misc :
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ClientSampleId :
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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
2-Pentanone, 4-...	5.069	5.2	ng	102470	1	7.948	395528	20.0
Hexadecane	23.906	2.9	ng	233375	6	24.717	1616400	20.0
Docosane, 11-de...	24.852	4.1	ng	330696	6	24.717	1616400	20.0
Octacosane	25.968	4.0	ng	322533	6	24.717	1616400	20.0
Heptadecane, 9-...	27.308	4.8	ng	384535	6	24.717	1616400	20.0
Eicosane, 2-met...	28.941	3.5	ng	281928	6	24.717	1616400	20.0
Hexadecane, 2-m...	30.898	2.9	ng	234063	6	24.717	1616400	20.0