LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG050124\
Data File : BG061080.D
Acq On : 1 May 2024 17:28
Operator : MA/JU
Sample : P2330-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
B-1(0.5-1.5)

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-BG043024.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG061080.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.159	23	29	37	rBV	23628	43387	2.58%	0.434%
2	3.676	113	117	125	rVB	11180	17320	1.03%	0.173%
3	5.526	424	432	444	rBV	414282	658818	39.20%	6.593%
4	7.107	692	701	712	rBV	418720	739916	44.02%	7.405%
5	7.935	834	842	849	rBV	121762	198956	11.84%	1.991%
6	9.087	1028	1038	1047	rBB	270106	466052	27.73%	4.664%
7	10.726	1311	1317	1324	rBV	140662	252060	15.00%	2.523%
8	13.182	1728	1735	1742	rBV	735032	1109604	66.02%	11.105%
9	14.222	1906	1912	1918	rBV4	16036	23678	1.41%	0.237%
10	14.563	1963	1970	1976	rBV	243059	376074	22.38%	3.764%
11	14.780	1997	2007	2013	rBV5	11797	28958	1.72%	0.290%
12	16.049	2217	2223	2232	rBV	712509	1026828	61.10%	10.277%
13	17.307	2429	2437	2442	rBV	283969	457438	27.22%	4.578%
14	17.354	2442	2445	2449	rVB	53644	69731	4.15%	0.698%
15	17.442	2455	2460	2464	rVB2	12029	17928	1.07%	0.179%
16	18.212	2584	2591	2600	rBV2	123889	204072	12.14%	2.042%
17	18.382	2615	2620	2632	rVB5	24628	62388	3.71%	0.624%
18	19.363	2779	2787	2793	rBV	148167	226980	13.51%	2.272%
19	19.422	2793	2797	2802	rBV2	39795	53798	3.20%	0.538%
20	19.481	2804	2807	2811	rBV2	50341	64396	3.83%	0.644%
21	19.610	2826	2829	2835	rBV8	12869	19597	1.17%	0.196%
22	19.722	2840	2848	2856	rVB	117353	211750	12.60%	2.119%
23	19.927	2878	2883	2890	rBV	1324101	1680677	100.00%	16.820%
24	20.221	2929	2933	2936	rBV2	27202	36379	2.16%	0.364%
25	21.237	3102	3106	3113	rVB2	85980	135117	8.04%	1.352%
26	21.561	3155	3161	3167	rBV2	296737	544623	32.40%	5.451%
27	22.377	3297	3300	3301	rBV2	37222	45620	2.71%	0.457%
28	23.834	3543	3548	3553	rVB	105067	197169	11.73%	1.973%
29	24.369	3633	3639	3649	rVB5	147604	354962	21.12%	3.552%
30	24.686	3687	3693	3702	rVB	165417	386658	23.01%	3.870%
31	25.856	3886	3892	3902	rVB3	99099	281052	16.72%	2.813%

Sum of corrected areas: 9991986

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG050124\
Data File : BG061080.D
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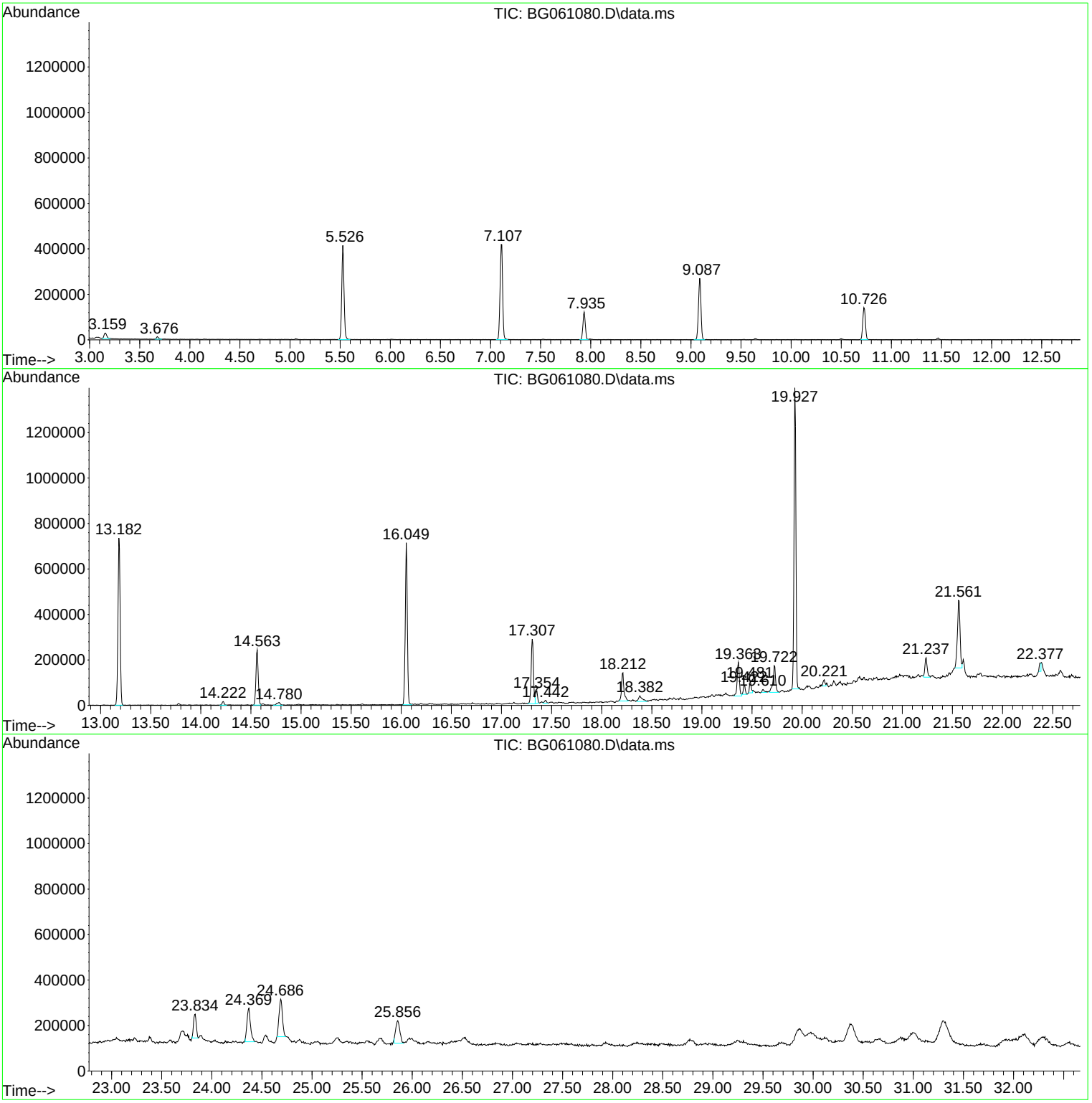
Operator : MA/JU
Sample : P2330-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
B-1(0.5-1.5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.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 : BG061080.D
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

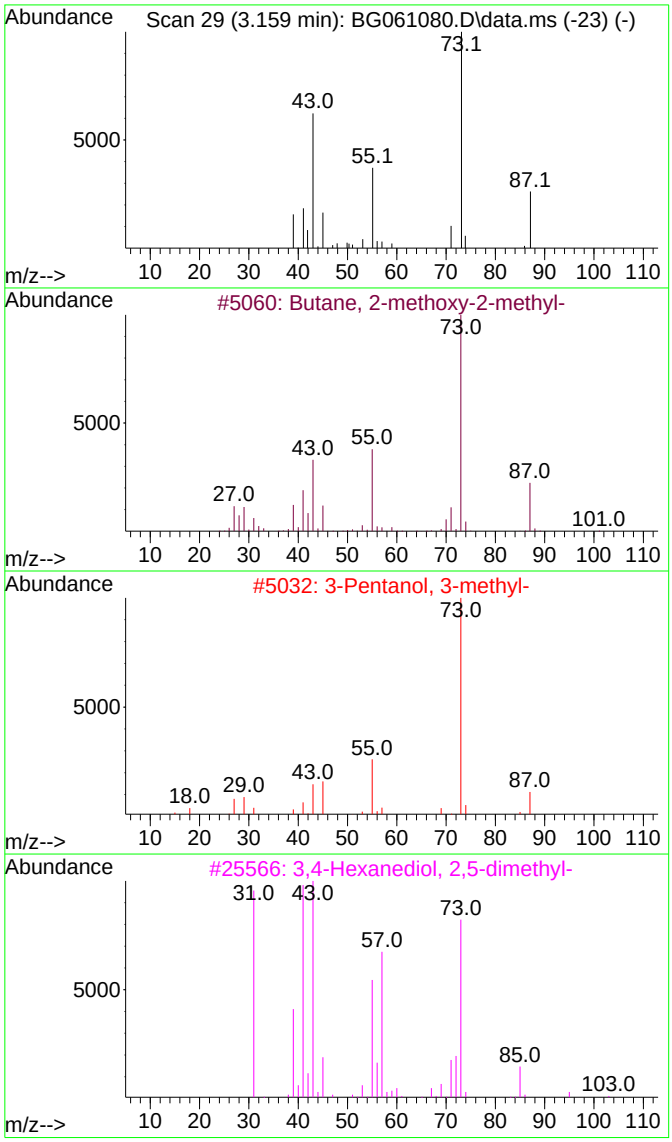
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

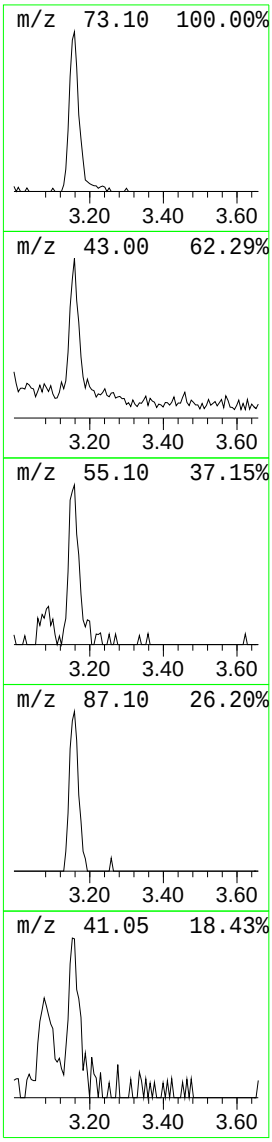
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.159	4.36 ng	43387	1,4-Dichlorobenzene-d4	7.935

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	28
3	3,4-Hexanediol, 2,5-dimethyl-	146	C8H18O2	022607-11-0	23
4	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	12
5	2-Butanone, 3-methoxy-3-methyl-	116	C6H12O2	036687-98-6	12





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Data File : BG061080.D
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Operator : MA/JU
Sample : P2330-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
B-1(0.5-1.5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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TIC Integration Parameters: LSCINT.P

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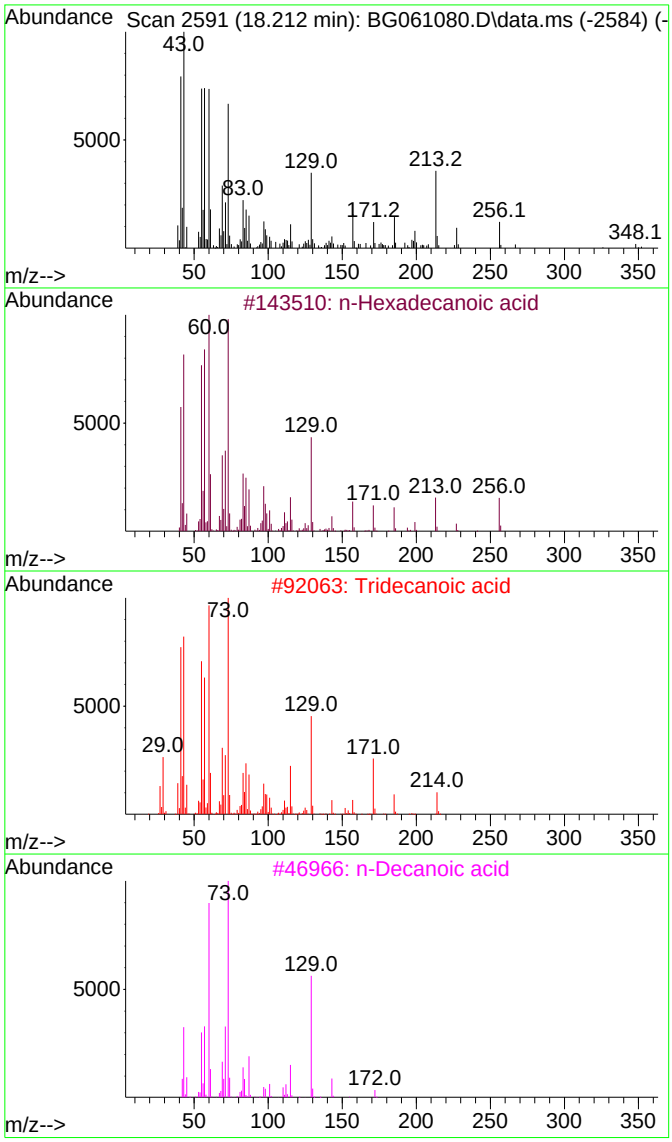
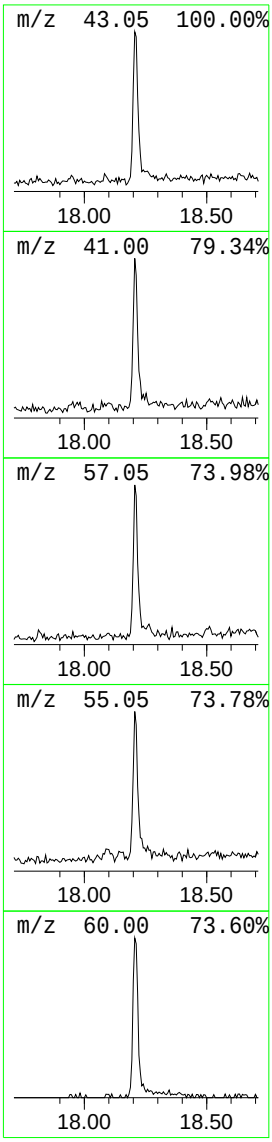
Peak Number 2 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.212	8.92 ng	204072	Phenanthrene-d10	17.307

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	70
3	n-Decanoic acid	172	C10H20O2	000334-48-5	60
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	58
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	52





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG050124\
Data File : BG061080.D
Acq On : 1 May 2024 17:28
Operator : MA/JU
Sample : P2330-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
B-1(0.5-1.5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.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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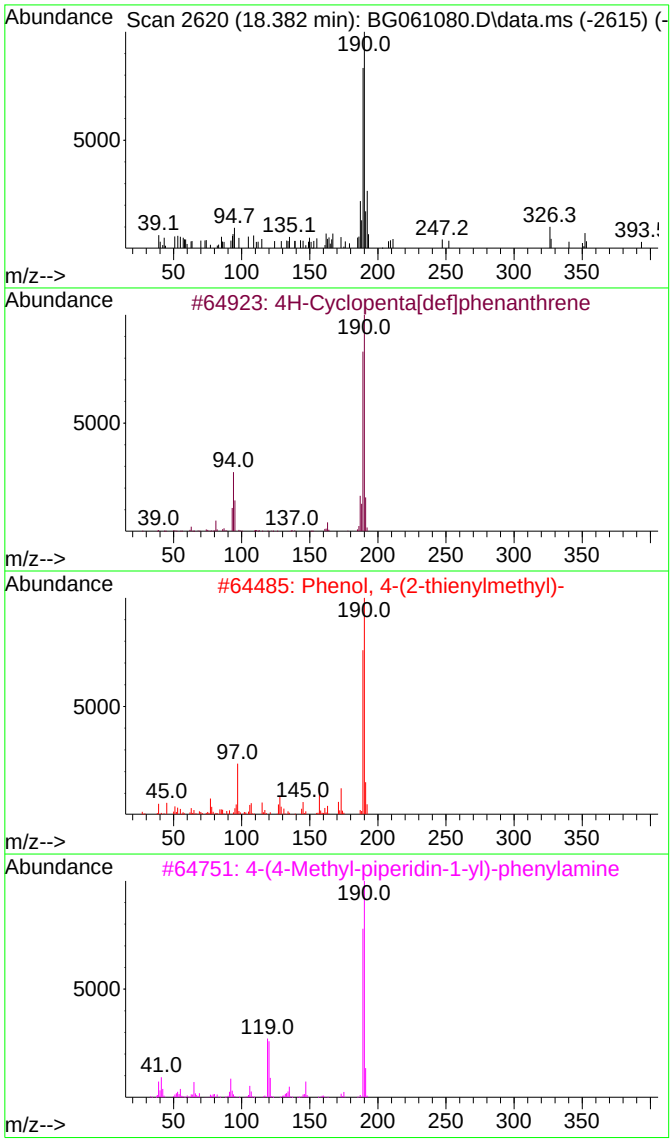
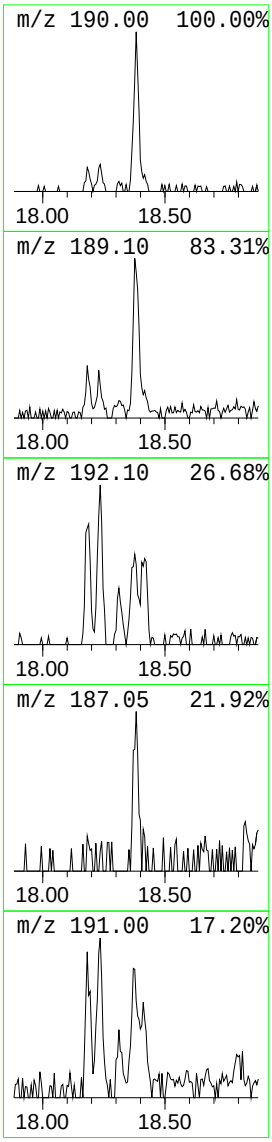
Peak Number 3 4H-Cyclopenta[def]phenanthrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.382	2.73 ng	62388	Phenanthrene-d10	17.307

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	74
2	Phenol, 4-(2-thienylmethyl)-	190	C11H10OS	091680-55-6	58
3	4-(4-Methyl-piperidin-1-yl)-phen...	190	C12H18N2	342013-25-6	52
4	Carbonic acid, ethyl 2-formyl-4,...	262	C10H8Cl2O4	1000331-34-4	50
5	Pyrazole-4-carboxaldehyde, 3-(4-...	190	C10H7FN2O	306936-57-2	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG050124\
Data File : BG061080.D
Acq On : 1 May 2024 17:28
Operator : MA/JU
Sample : P2330-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
B-1(0.5-1.5)

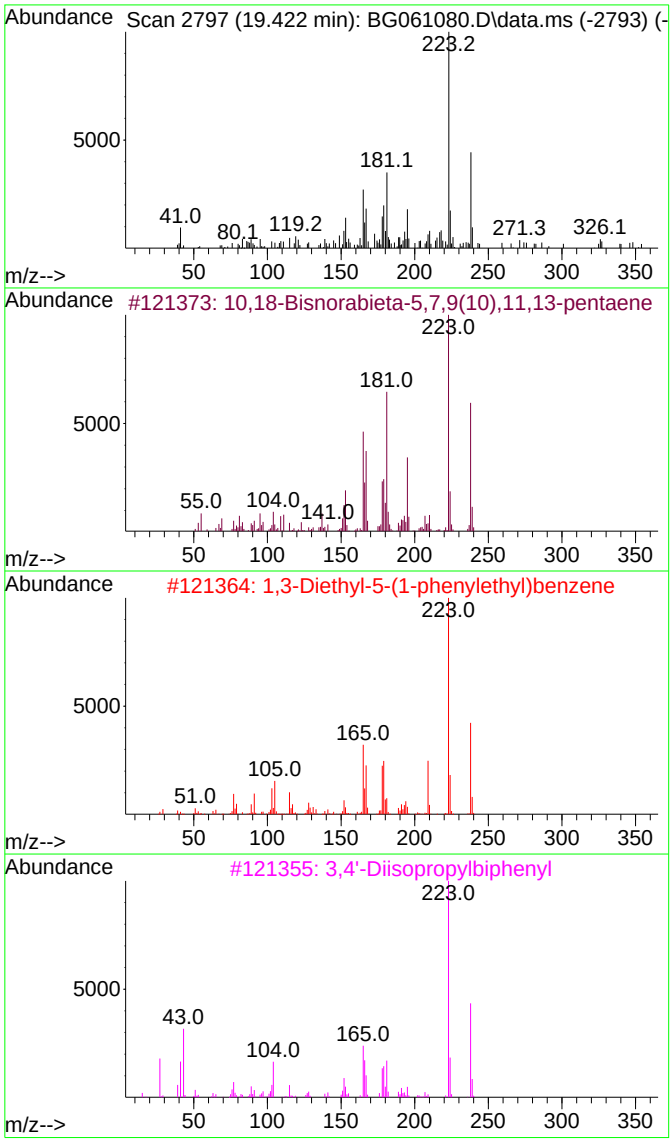
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

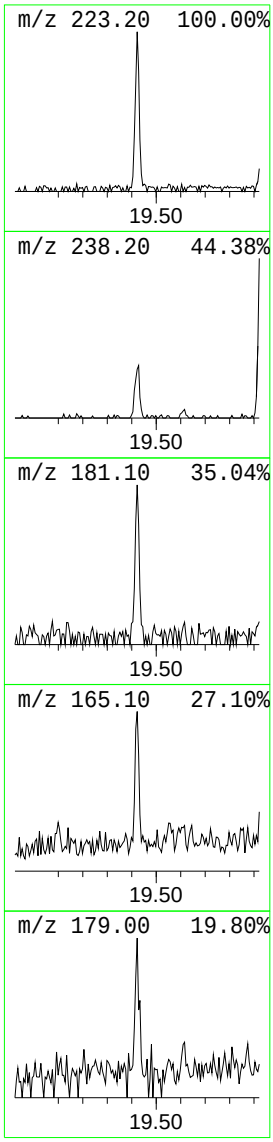
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 10,18-Bisnorabieta-5,7,9(10... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.422	2.35 ng	53798	Phenanthrene-d10	17.307

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	10,18-Bisnorabieta-5,7,9(10),11,...	238	C18H22	006566-19-4	97
2	1,3-Diethyl-5-(1-phenylethyl)ben...	238	C18H22	1000482-32-6	91
3	3,4'-Diisopropylbiphenyl	238	C18H22	061434-46-6	81
4	4,4'-Diisopropylbiphenyl	238	C18H22	018970-30-4	80
5	Benzene, 2-chloro-1,3,5-tris(1-m...	238	C15H23Cl	055538-62-0	68





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG050124\
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Acq On : 1 May 2024 17:28
Operator : MA/JU
Sample : P2330-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
B-1(0.5-1.5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
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TIC Library : C:\Database\NIST20.L
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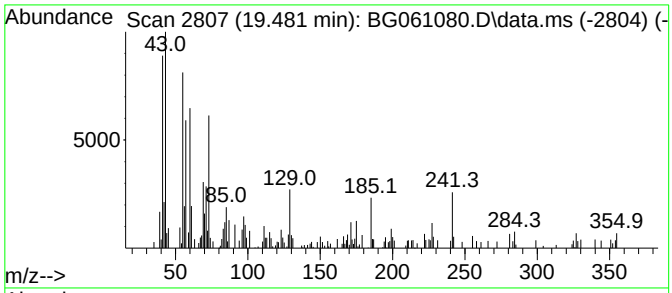
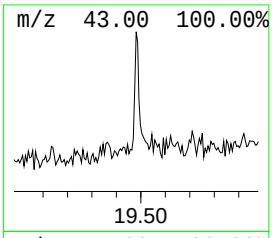
****

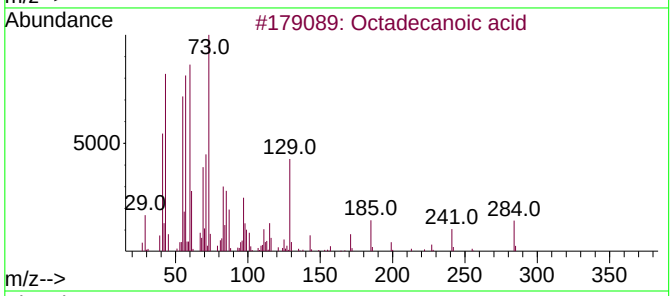
Peak Number 5 Octadecanoic acid Concentration Rank 8

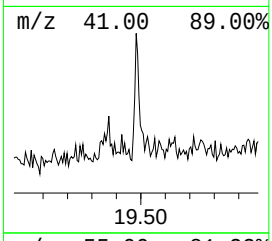
R.T.	EstConc	Area	Relative to ISTD	R.T.
19.481	2.36 ng	64396	Chrysene-d12	21.566

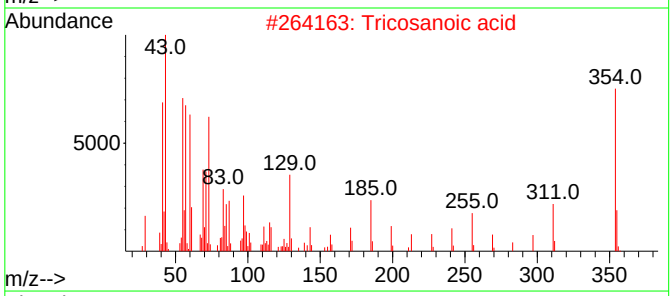
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	78
2	Tricosanoic acid	354	C23H46O2	002433-96-7	58
3	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	50
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	49
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	49

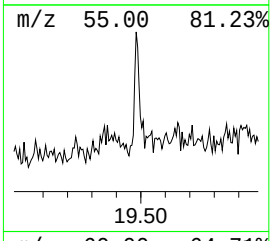


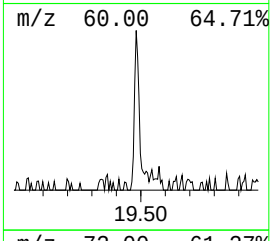


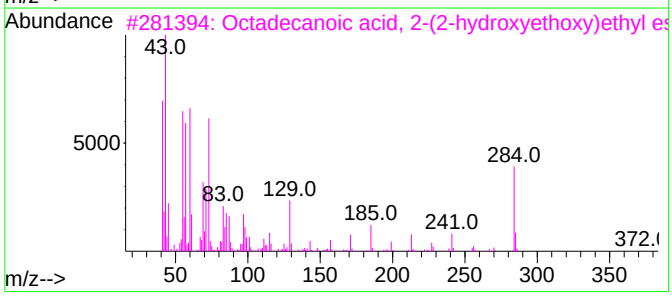


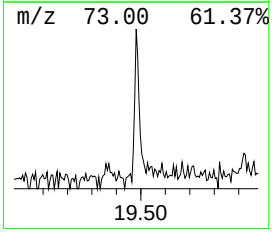












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Instrument :
BNA_G
ClientSampleId :
B-1(0.5-1.5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

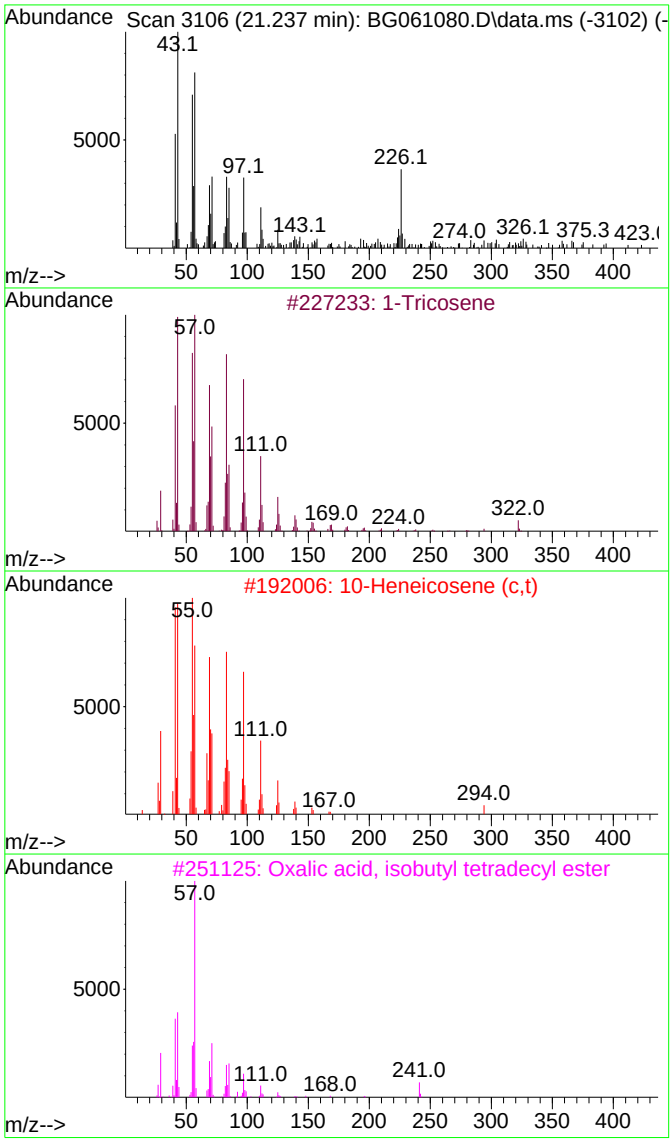
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

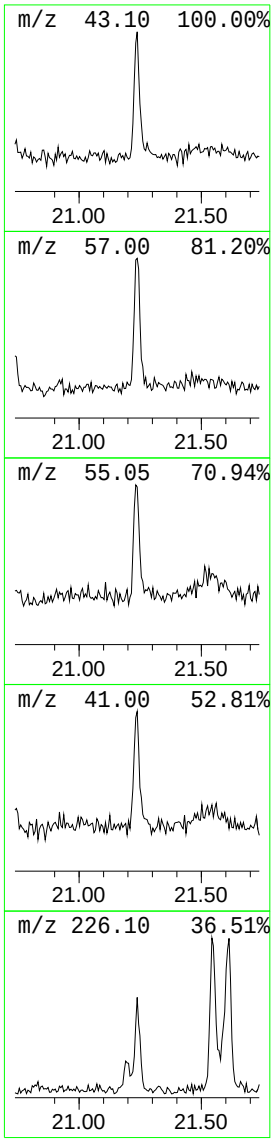
****

Peak Number 6 1-Tricosene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.237	4.96 ng	135117	Chrysene-d12	21.566

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tricosene	322	C23H46	018835-32-0	78
2	10-Heneicosene (c,t)	294	C21H42	095008-11-0	48
3	Oxalic acid, isobutyl tetradecyl...	342	C20H38O4	1000309-37-9	41
4	1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	41
5	Oxalic acid, allyl octadecyl ester	382	C23H42O4	1000309-24-5	41





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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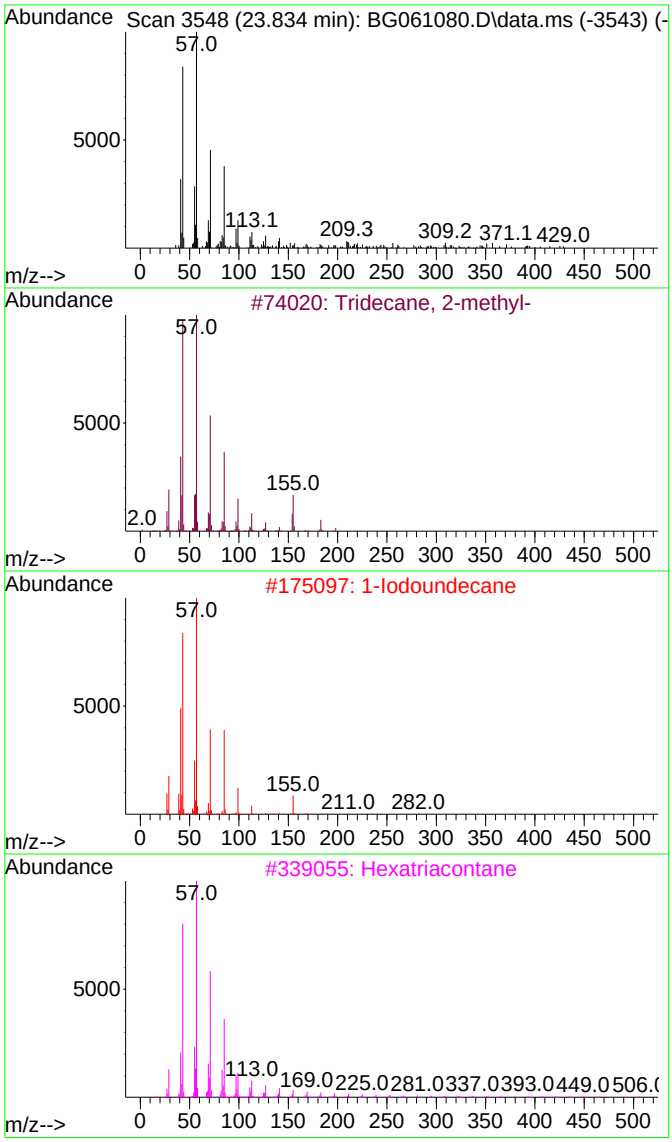
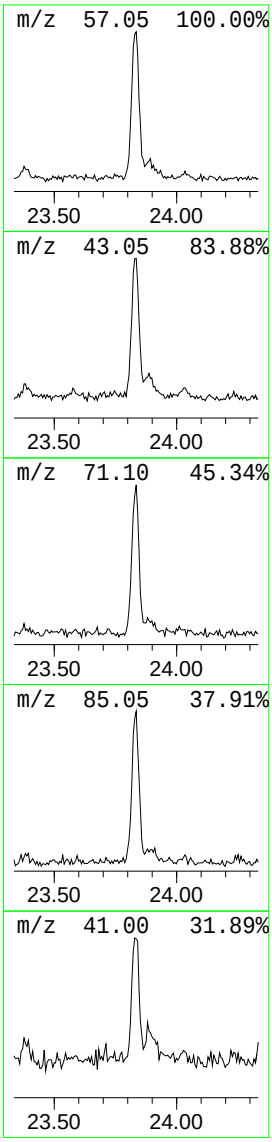
Peak Number 7 Tridecane, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.834	10.20 ng	197169	Perylene-d12	24.686

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane, 2-methyl-	198	C14H30	001560-96-9	87
2	1-Iodoundecane	282	C11H23I	004282-44-4	83
3	Hexatriacontane	507	C36H74	000630-06-8	83
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	80
5	Heptacosane	380	C27H56	000593-49-7	80





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Data File : BG061080.D
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Operator : MA/JU
Sample : P2330-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
B-1(0.5-1.5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.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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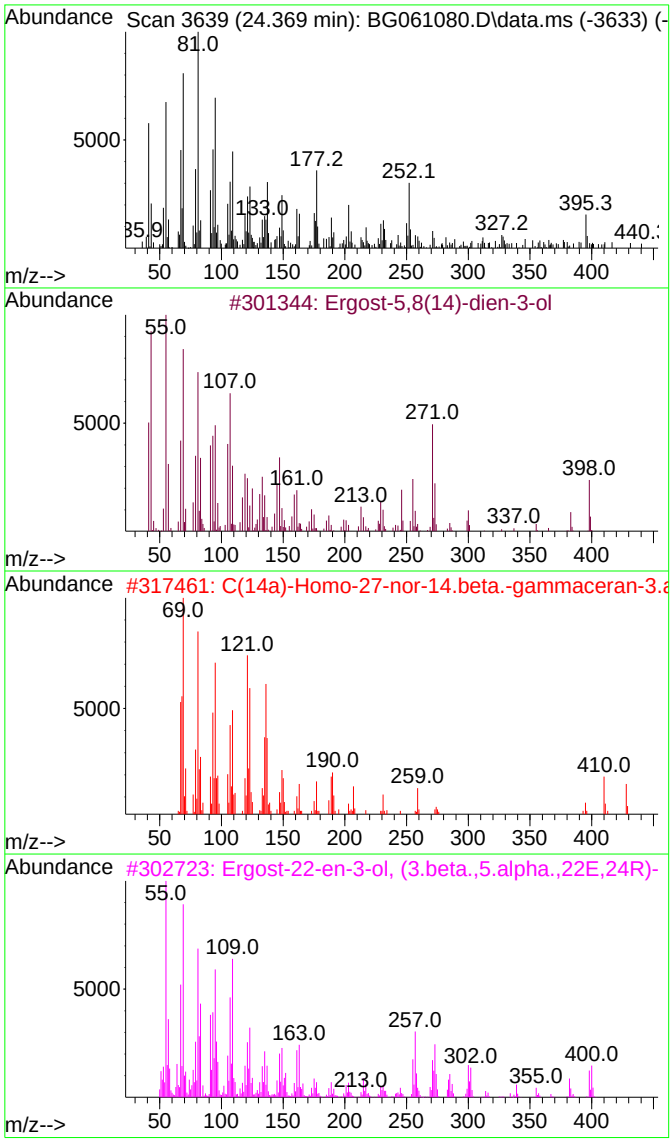
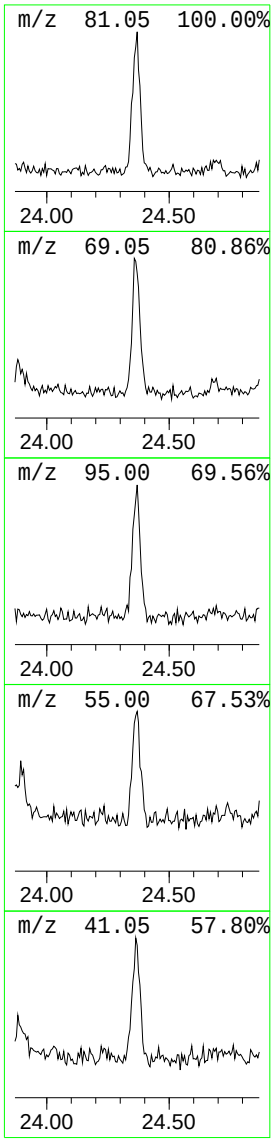
Peak Number 8 unknown24.369 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.369	18.36 ng	354962	Perylene-d12	24.686

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ergost-5,8(14)-dien-3-ol	398	C28H46O	177962-83-3	34
2	C(14a)-Homo-27-nor-14.beta.-gamm...	428	C30H52O	024739-08-0	32
3	Ergost-22-en-3-ol, (3.beta.,5.al...	400	C28H48O	036422-25-0	32
4	2,6,11,15-Tetramethyl-hexadeca-2...	272	C20H32	038259-79-9	27
5	9,19-Cycloergost-24(28)-en-3-ol,...	426	C30H50O	000469-39-6	23





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG050124\
Data File : BG061080.D
Acq On : 1 May 2024 17:28
Operator : MA/JU
Sample : P2330-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
B-1(0.5-1.5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

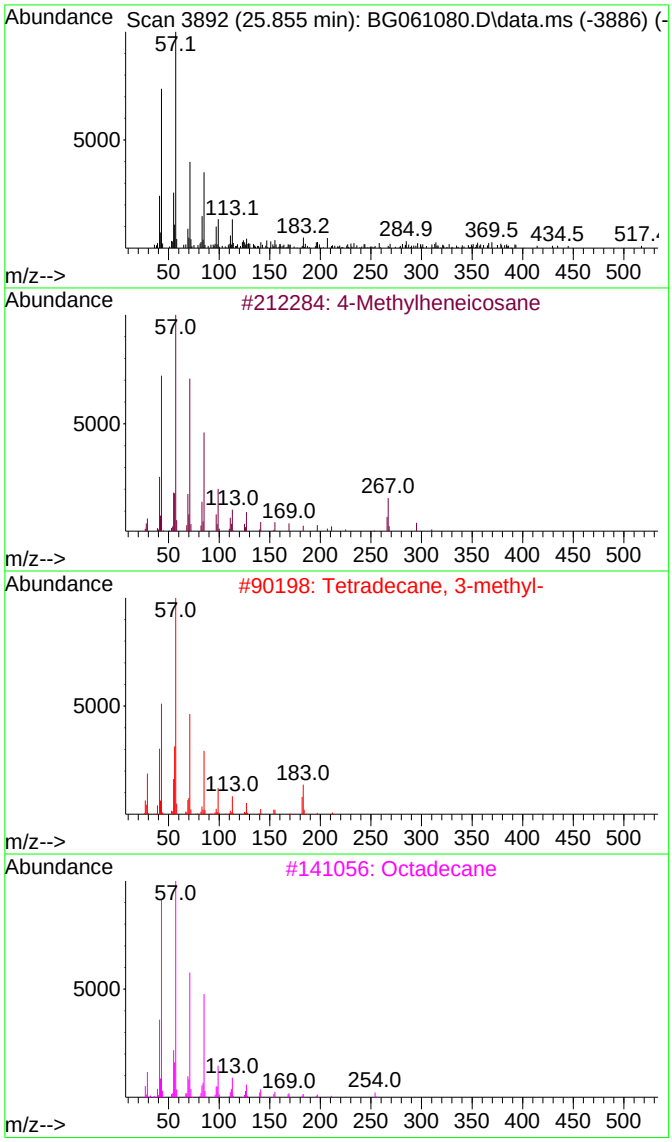
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

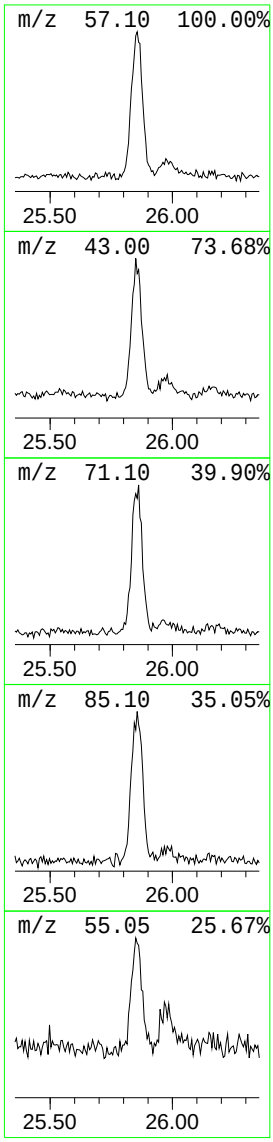
****

Peak Number 9 4-Methylheneicosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.855	14.54 ng	281052	Perylene-d12	24.686

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Methylheneicosane	310	C22H46	025117-29-7	76
2	Tetradecane, 3-methyl-	212	C15H32	018435-22-8	76
3	Octadecane	254	C18H38	000593-45-3	76
4	Heptadecane, 2-methyl-	254	C18H38	001560-89-0	68
5	Docosane	310	C22H46	000629-97-0	68





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG050124\
Data File : BG061080.D
Acq On : 1 May 2024 17:28
Operator : MA/JU
Sample : P2330-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
B-1(0.5-1.5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.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
Butane, 2-metho...	3.159	4.4	ng	43387	1	7.935	198956	20.0
n-Hexadecanoic ...	18.212	8.9	ng	204072	4	17.307	457438	20.0
4H-Cyclopenta[d...	18.382	2.7	ng	62388	4	17.307	457438	20.0
10,18-Bisnorabi...	19.422	2.4	ng	53798	4	17.307	457438	20.0
Octadecanoic acid	19.481	2.4	ng	64396	5	21.566	544623	20.0
1-Tricosene	21.237	5.0	ng	135117	5	21.566	544623	20.0
Tridecane, 2-me...	23.834	10.2	ng	197169	6	24.686	386658	20.0
unknown24.369	24.369	18.4	ng	354962	6	24.686	386658	20.0
4-Methylheneico...	25.855	14.5	ng	281052	6	24.686	386658	20.0