LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062123\
Data File : BG057789.D
Acq On : 21 Jun 2023 18:03
Operator : CG/JU
Sample : 03289-10
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-04-12.0-14.0

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-BG061923.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG057789.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.027	325	330	339	rVB	83124	120433	7.22%	1.121%
2	5.491	403	409	418	rVB	346414	532222	31.89%	4.954%
3	7.084	671	680	689	rBV	355991	598756	35.88%	5.573%
4	7.924	816	823	830	rVB	95886	154206	9.24%	1.435%
5	9.081	1011	1020	1029	rBV	207791	354218	21.22%	3.297%
6	10.726	1292	1300	1308	rBV	138648	248743	14.90%	2.315%
7	13.182	1710	1718	1726	rBV	555811	858307	51.43%	7.989%
8	14.451	1929	1934	1939	rVB	16501	21365	1.28%	0.199%
9	14.557	1944	1952	1959	rVB	251638	388263	23.26%	3.614%
10	15.403	2091	2096	2102	rVB	27175	32308	1.94%	0.301%
11	15.909	2177	2182	2188	rVB	79970	116117	6.96%	1.081%
12	16.044	2195	2205	2212	rBV	534607	826764	49.54%	7.696%
13	16.261	2238	2242	2246	rBV	32288	51465	3.08%	0.479%
14	17.054	2373	2377	2382	rBV	33414	41907	2.51%	0.390%
15	17.107	2382	2386	2391	rVB	14244	21232	1.27%	0.198%
16	17.301	2413	2419	2424	rBV	377348	564837	33.84%	5.258%
17	17.795	2498	2503	2508	rBV	37817	49185	2.95%	0.458%
18	18.188	2565	2570	2584	rBV	215457	355384	21.29%	3.308%
19	18.488	2618	2621	2630	rVB	38265	53304	3.19%	0.496%
20	19.117	2725	2728	2732	rVB	29763	31299	1.88%	0.291%
21	19.352	2760	2768	2776	rBV2	42703	80047	4.80%	0.745%
22	19.463	2783	2787	2796	rBV	108670	172402	10.33%	1.605%
23	19.604	2808	2811	2816	rBV3	13728	17740	1.06%	0.165%
24	19.710	2823	2829	2834	rVB2	31895	65227	3.91%	0.607%
25	19.916	2858	2864	2872	rVB	1319497	1668987	100.00%	15.535%
26	20.221	2914	2916	2920	rVB2	16884	20832	1.25%	0.194%
27	21.167	3072	3077	3081	rBV	115019	214506	12.85%	1.997%
28	21.226	3081	3087	3092	rVV2	181846	432747	25.93%	4.028%
29	21.290	3092	3098	3107	rVB	779661	1049038	62.85%	9.765%
30	21.367	3108	3111	3115	rBV	35993	49833	2.99%	0.464%
31	21.555	3136	3143	3148	rVB	363062	611296	36.63%	5.690%
32	21.755	3173	3177	3181	rVB2	33942	44181	2.65%	0.411%
33	22.354	3275	3279	3287	rVB3	33078	66023	3.96%	0.615%
34	23.218	3422	3426	3433	rVB2	45259	77436	4.64%	0.721%
35	24.704	3670	3679	3696	rVB	249744	752759	45.10%	7.007%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062123\
Data File : BG057789.D
Acq On : 21 Jun 2023 18:03
Operator : CG/JU
Sample : 03289-10
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-04-12.0-14.0

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-BG061923.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

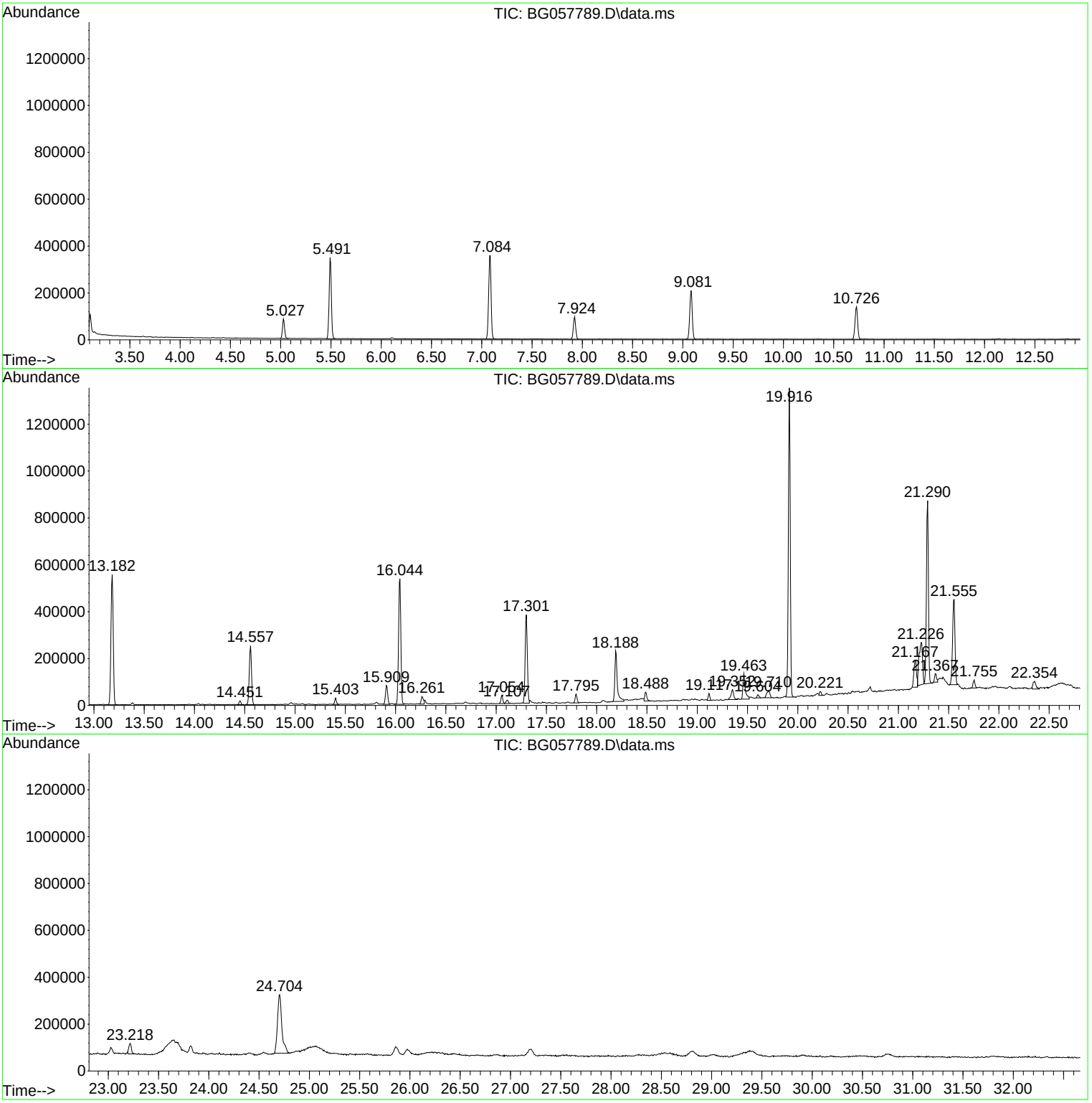
Sum of corrected areas: 10743369

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062123\
Data File : BG057789.D
Acq On : 21 Jun 2023 18:03
Operator : CG/JU
Sample : 03289-10
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-04-12.0-14.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.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\BG062123\
Data File : BG057789.D
Acq On : 21 Jun 2023 18:03
Operator : CG/JU
Sample : 03289-10
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-04-12.0-14.0

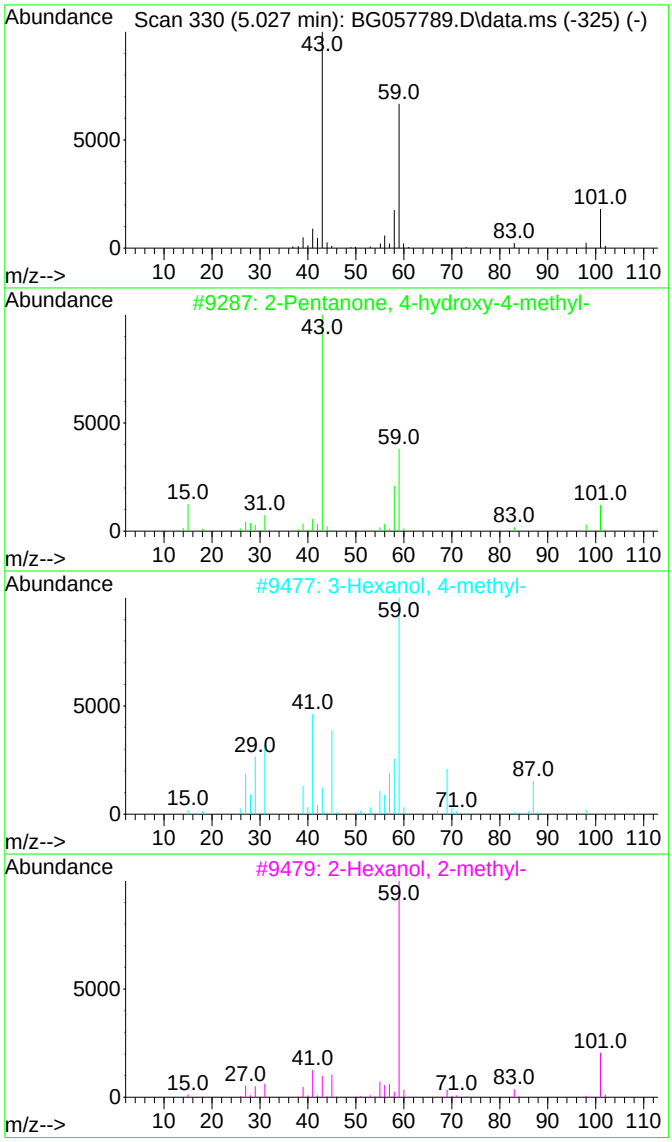
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

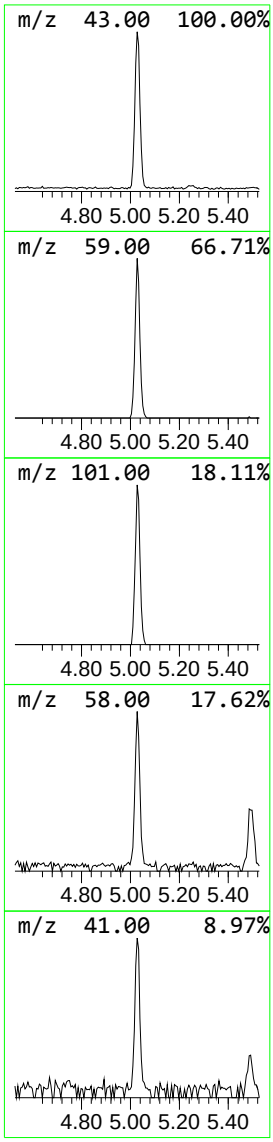
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.027	15.62 ng	120433	1,4-Dichlorobenzene-d4	7.924

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062123\
Data File : BG057789.D
Acq On : 21 Jun 2023 18:03
Operator : CG/JU
Sample : 03289-10
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-04-12.0-14.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

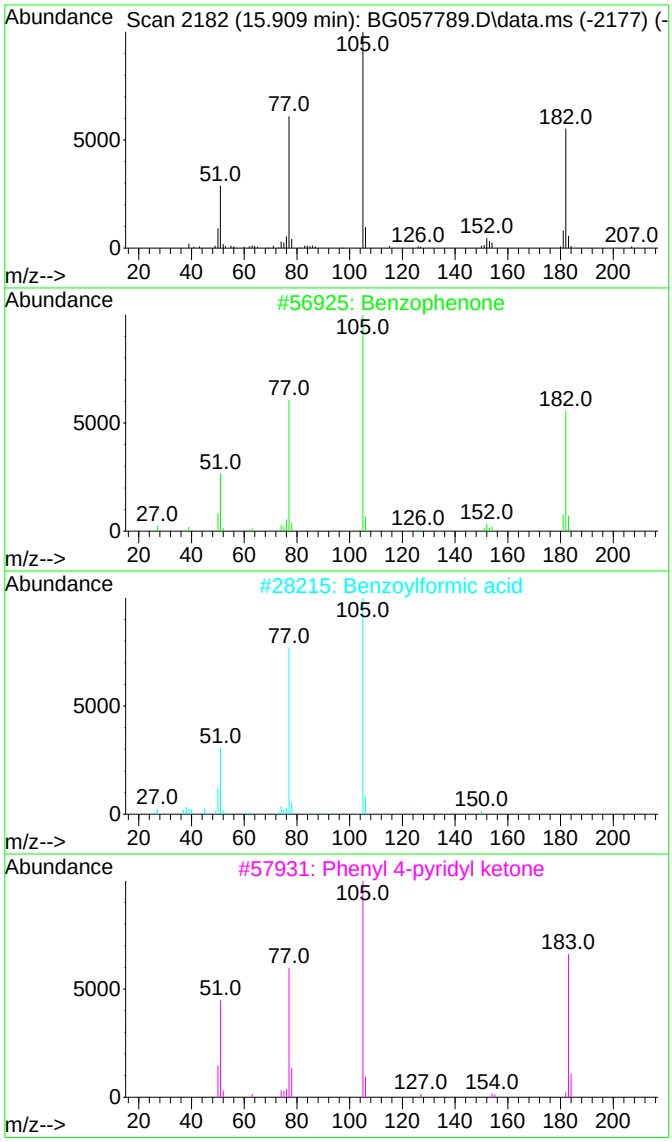
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

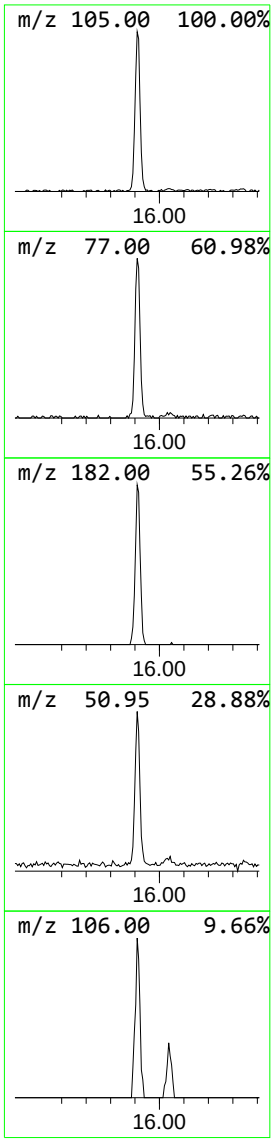
****

Peak Number 2 Benzophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.909	5.98 ng	116117	Acenaphthene-d10	14.557

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	97
2	Benzoylformic acid	150	C8H6O3	000611-73-4	64
3	Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	58
4	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	52
5	Phenylglyoxal	134	C8H6O2	001074-12-0	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062123\
Data File : BG057789.D
Acq On : 21 Jun 2023 18:03
Operator : CG/JU
Sample : 03289-10
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-04-12.0-14.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

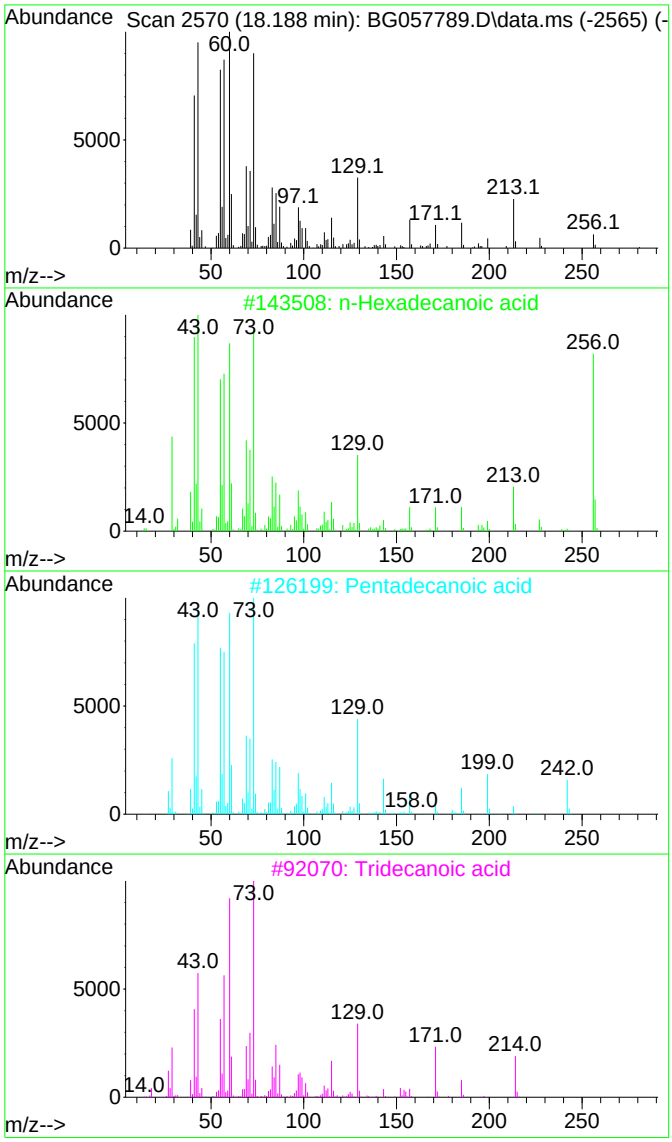
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

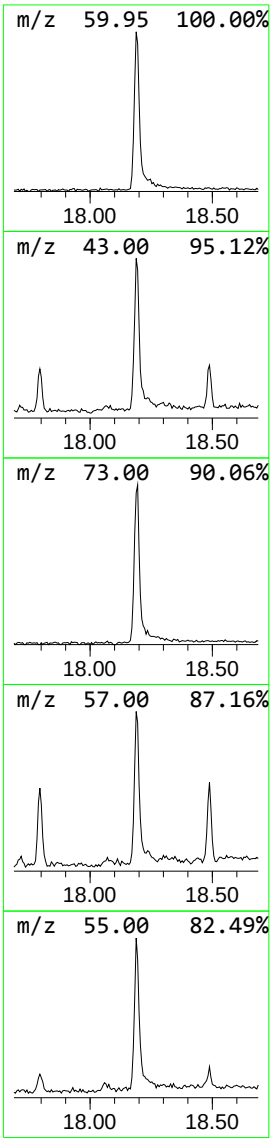
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.188	12.58 ng	355384	Phenanthrene-d10	17.301

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Tridecanoic acid	214	C13H26O2	000638-53-9	83
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Dodecanoic acid	200	C12H24O2	000143-07-7	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062123\
Data File : BG057789.D
Acq On : 21 Jun 2023 18:03
Operator : CG/JU
Sample : 03289-10
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-04-12.0-14.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

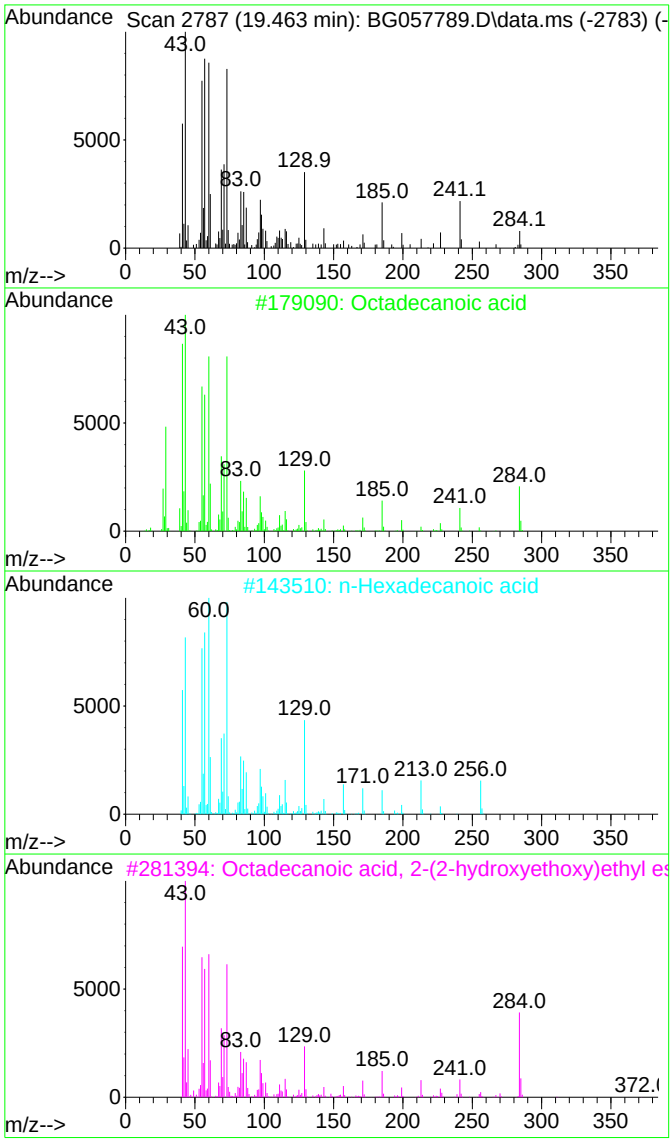
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

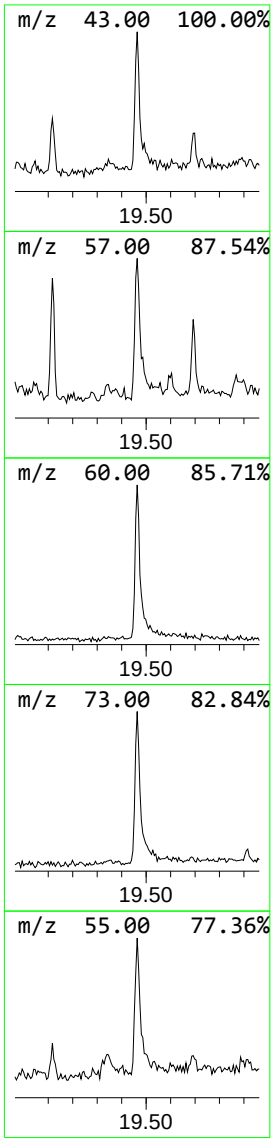
****

Peak Number 5 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.463	5.64 ng	172402	Chrysene-d12	21.555

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	91
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
3	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	86
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5	n-Decanoic acid	172	C10H20O2	000334-48-5	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062123\
Data File : BG057789.D
Acq On : 21 Jun 2023 18:03
Operator : CG/JU
Sample : 03289-10
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-04-12.0-14.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

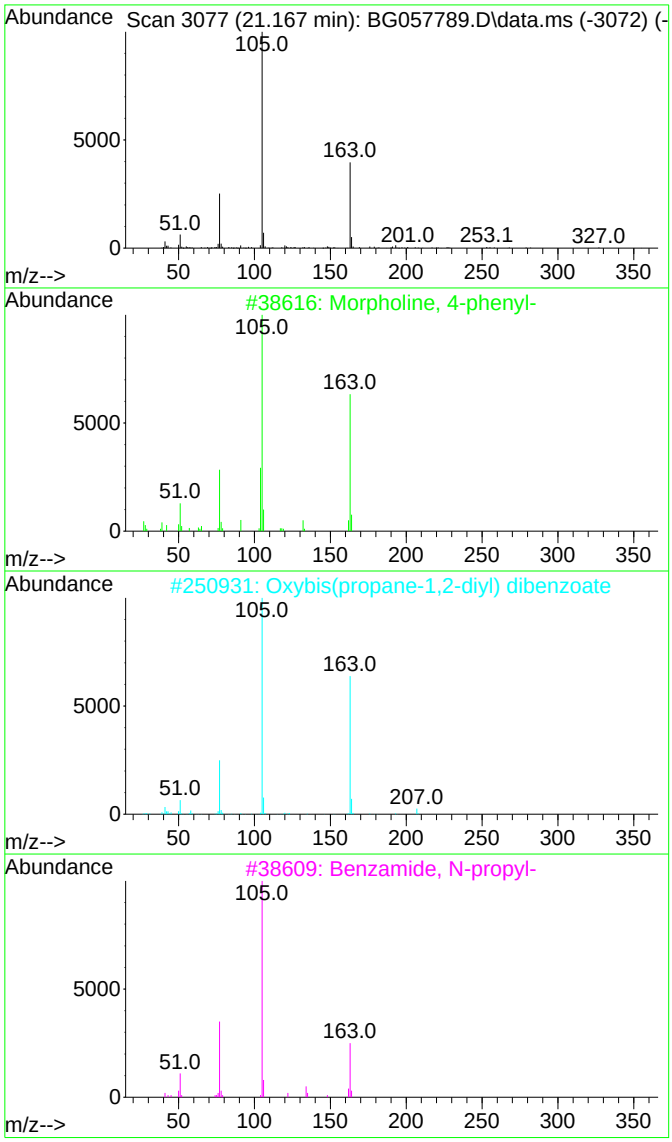
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

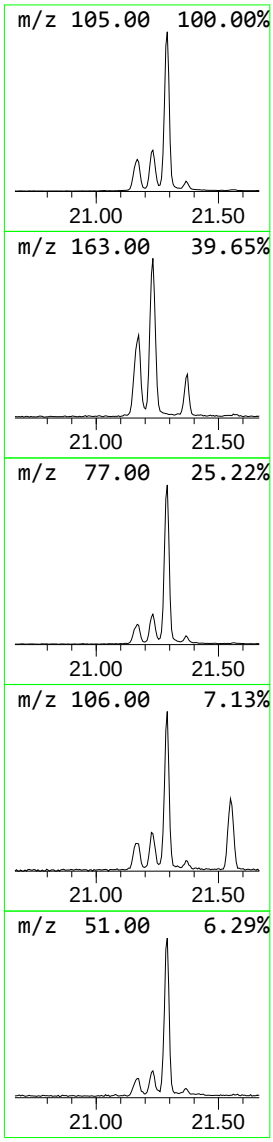
****

Peak Number 7 Morpholine, 4-phenyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.167	7.02 ng	214506	Chrysene-d12	21.555

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	72
2	Oxybis(propane-1,2-diyl) dibenzoate	342	C20H22O5	000094-03-1	72
3	Benzamide, N-propyl-	163	C10H13NO	010546-70-0	43
4	5(4H)-Oxazolone, 4-[(4-methoxyph...	279	C17H13NO3	005429-22-1	35
5	Phenylglyoxylic acid, butyl ester	206	C12H14O3	1000453-46-6	30





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062123\
Data File : BG057789.D
Acq On : 21 Jun 2023 18:03
Operator : CG/JU
Sample : 03289-10
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-04-12.0-14.0

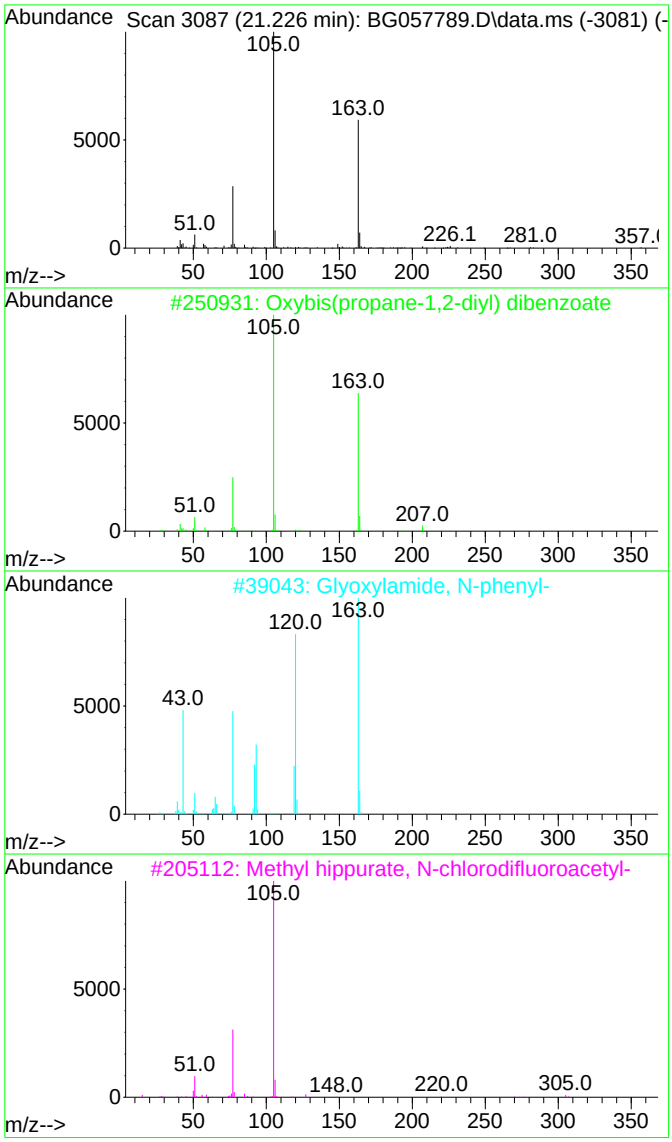
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

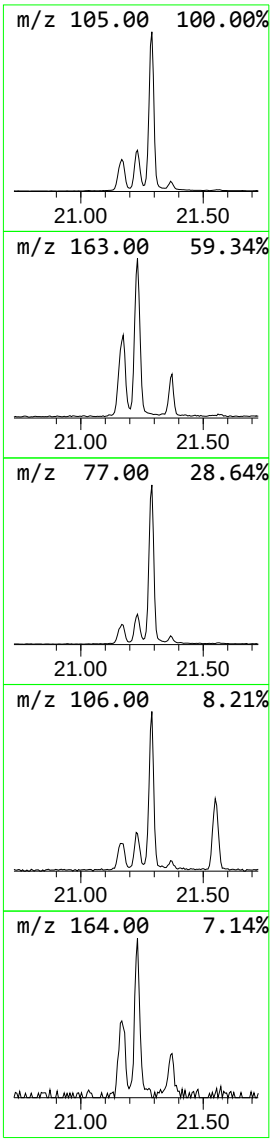
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Oxybis(propane-1,2-diyl) di... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.226	14.16 ng	432747	Chrysene-d12	21.555

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxybis(propane-1,2-diyl) dibenzoate	342	C20H22O5	000094-03-1	80
2	Glyoxylamide, N-phenyl-	163	C9H9NO2	032331-52-5	47
3	Methyl hippurate, N-chlorodifluo...	305	C12H10ClF2NO4	1000446-92-2	35
4	benzamide, N-[4-[7-(benzoyloxy)-...	461	C29H19NO5	1010399-44-9	35
5	Benzeneacetic acid, .alpha.-oxo-...	178	C10H10O3	001603-79-8	27





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062123\
Data File : BG057789.D
Acq On : 21 Jun 2023 18:03
Operator : CG/JU
Sample : 03289-10
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-04-12.0-14.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

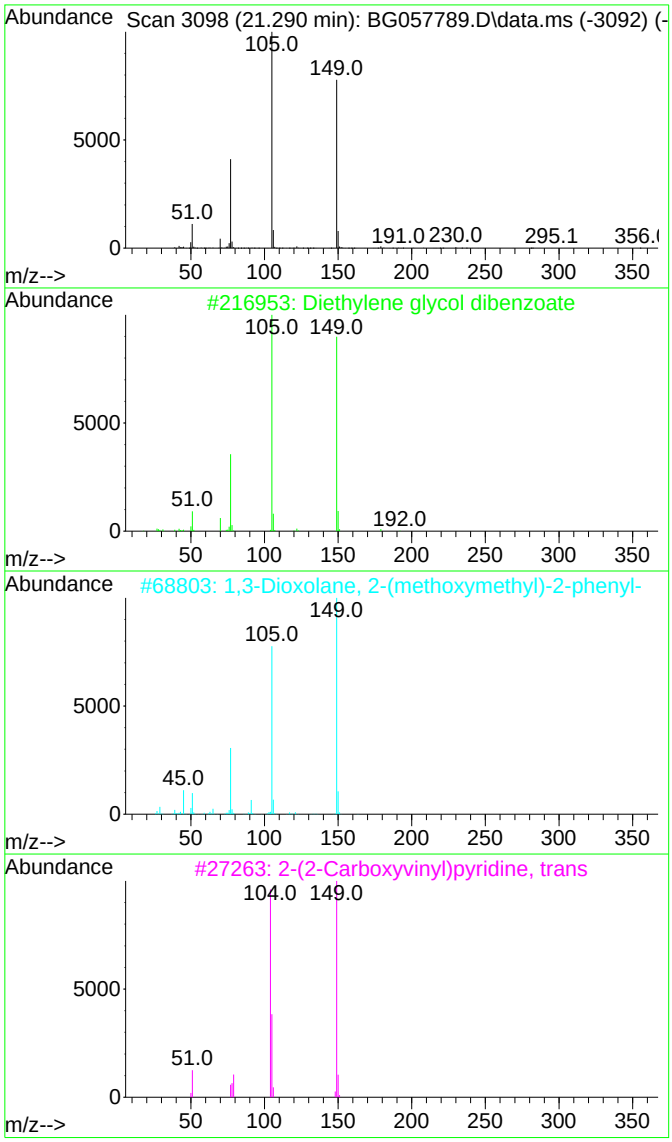
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

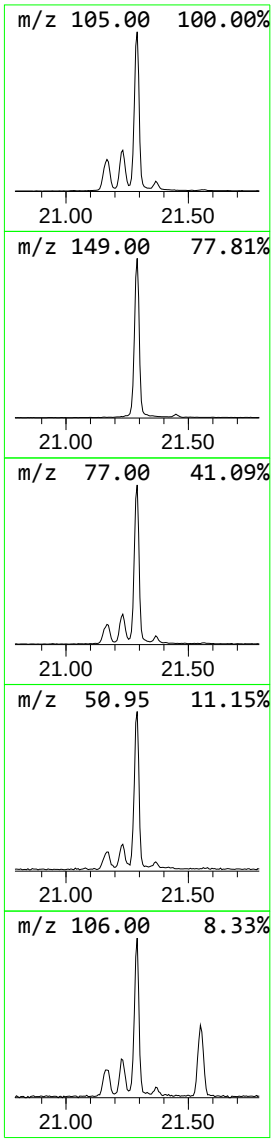
****

Peak Number 9 Diethylene glycol dibenzoate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.291	34.32 ng	1049040	Chrysene-d12	21.555

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	80
2	1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	59
3	2-(2-Carboxyvinyl)pyridine, trans	149	C8H7NO2	007340-22-9	49
4	2-Methyl-4-hydroxybenzoxazole	149	C8H7NO2	051110-60-2	43
5	3-(Benzoylthio)-2-methylpropanoi...	224	C11H12O3S	067714-34-5	35





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062123\
Data File : BG057789.D
Acq On : 21 Jun 2023 18:03
Operator : CG/JU
Sample : 03289-10
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-04-12.0-14.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

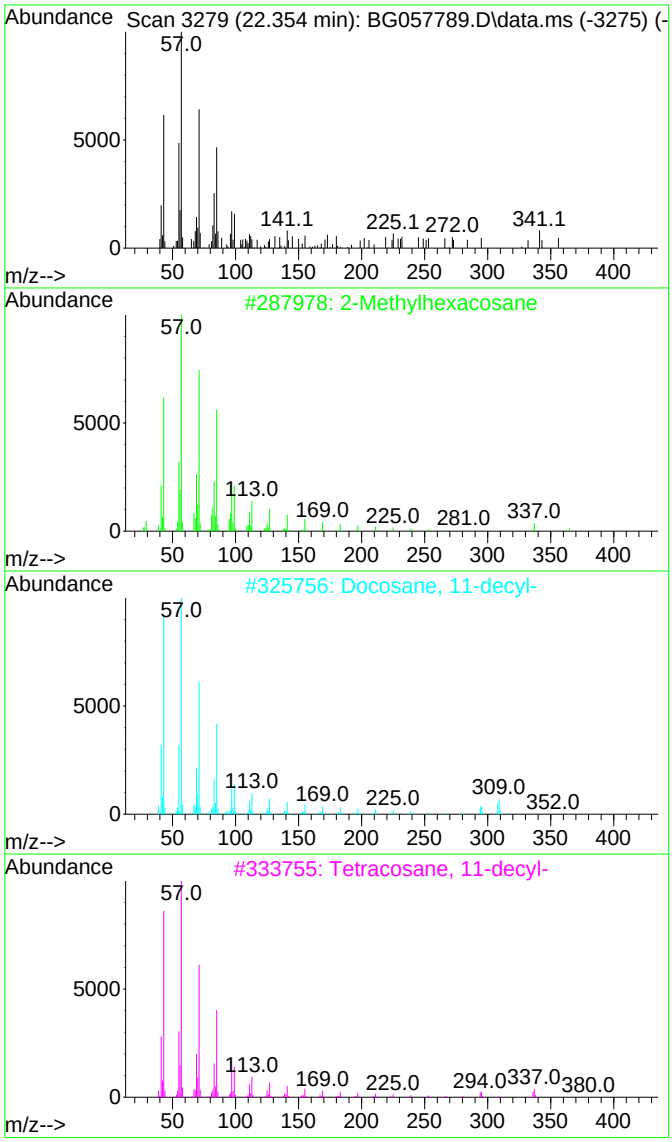
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

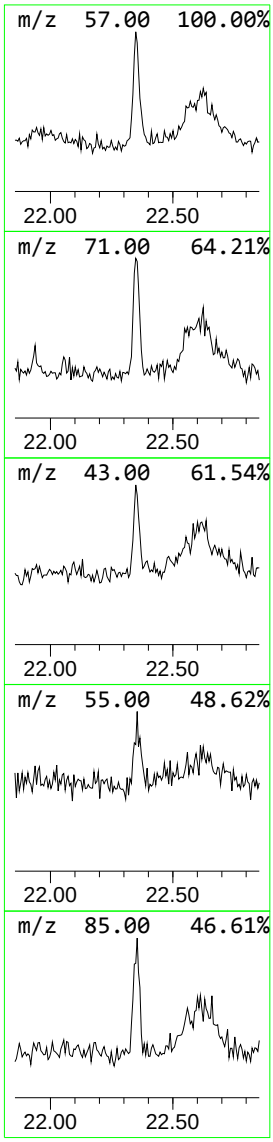
****

Peak Number 10 2-Methylhexacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.354	2.16 ng	66023	Chrysene-d12	21.555

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Methylhexacosane	380	C27H56	001561-02-0	58
2	Docosane, 11-decyl-	451	C32H66	055401-55-3	58
3	Tetracosane, 11-decyl-	479	C34H70	055429-84-0	58
4	Hentriacontane	437	C31H64	000630-04-6	52
5	Hexacosane	366	C26H54	000630-01-3	52





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062123\
Data File : BG057789.D
Acq On : 21 Jun 2023 18:03
Operator : CG/JU
Sample : 03289-10
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-04-12.0-14.0

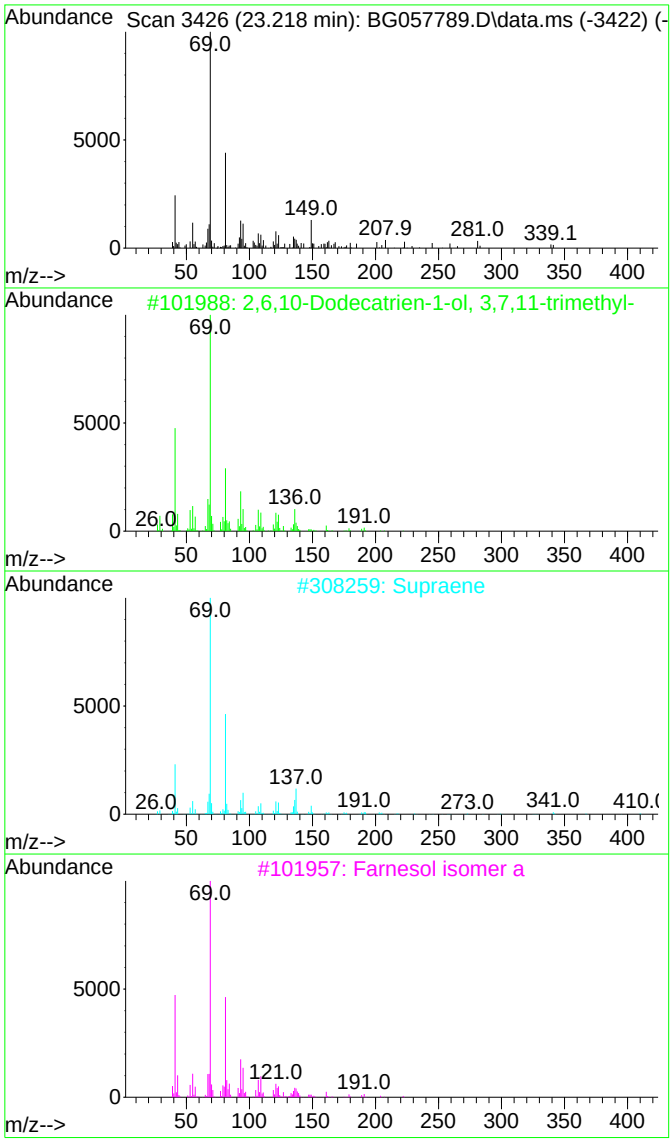
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

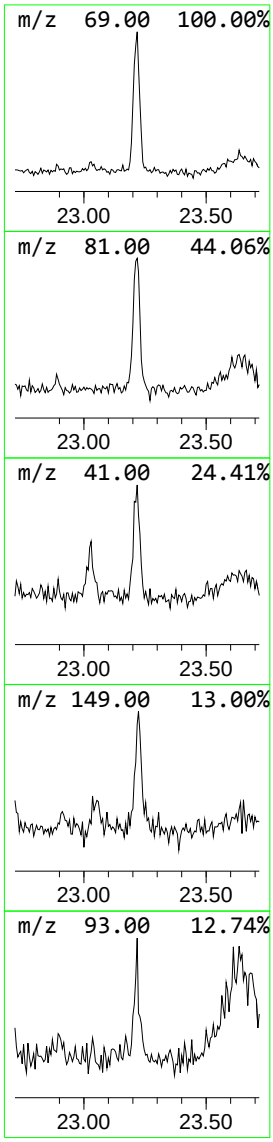
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 2,6,10-Dodecatrien-1-ol, 3,... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.218	2.06 ng	77436	Perylene-d12	24.704

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	64
2	Supraene	410	C30H50	007683-64-9	64
3	Farnesol isomer a	222	C15H26O	1000108-92-4	59
4	1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	53
5	Cyclopropanemethanol, 2-methyl-2...	168	C11H20O	098678-70-7	53





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062123\
Data File : BG057789.D
Acq On : 21 Jun 2023 18:03
Operator : CG/JU
Sample : 03289-10
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-04-12.0-14.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.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-...	5.027	15.6	ng	120433	1	7.924	154206	20.0
Benzophenone	15.909	6.0	ng	116117	3	14.557	388263	20.0
n-Hexadecanoic ...	18.188	12.6	ng	355384	4	17.301	564837	20.0
Octadecanoic acid	19.463	5.6	ng	172402	5	21.555	611296	20.0
Morpholine, 4-p...	21.167	7.0	ng	214506	5	21.555	611296	20.0
Oxybis(propane-...	21.226	14.2	ng	432747	5	21.555	611296	20.0
Diethylene glyc...	21.291	34.3	ng	1049040	5	21.555	611296	20.0
2-Methylhexacosane	22.354	2.2	ng	66023	5	21.555	611296	20.0
2,6,10-Dodecatr...	23.218	2.1	ng	77436	6	24.704	752759	20.0