Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011323\
Data File : BG056282.D
Acq On : 13 Jan 2023 17:57
Operator : CG/JU
Sample : O1135-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-2

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-BG122722.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG056282.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.331	3	7	19	rVB	181352	267063	8.93%	1.843%
2	5.358	345	352	360	rVB	121766	191291	6.40%	1.320%
3	5.834	426	433	446	rVB	498150	801892	26.83%	5.534%
4	7.449	699	708	716	rBV	519533	902016	30.18%	6.225%
5	8.319	849	856	862	rBV2	116944	199250	6.67%	1.375%
6	9.488	1046	1055	1063	rBV	300636	528768	17.69%	3.649%
7	11.151	1329	1338	1345	rBV	158952	285594	9.55%	1.971%
8	13.554	1738	1747	1756	rBV	1113086	1682379	56.28%	11.611%
9	14.929	1971	1981	1988	rBV	324237	509301	17.04%	3.515%
10	16.268	2203	2209	2215	rBV	386087	536491	17.95%	3.703%
11	16.404	2226	2232	2243	rBV	874784	1383900	46.30%	9.551%
12	16.827	2300	2304	2310	rVB	23990	33459	1.12%	0.231%
13	17.667	2440	2447	2451	rBV	449685	696328	23.29%	4.806%
14	17.708	2451	2454	2459	rVB	74964	104169	3.48%	0.719%
15	18.513	2584	2591	2598	rBV2	96094	164083	5.49%	1.132%
16	18.578	2598	2602	2609	rVB3	22506	42235	1.41%	0.291%
17	18.730	2620	2628	2632	rBV4	20481	45786	1.53%	0.316%
18	19.694	2787	2792	2797	rVB	137288	194789	6.52%	1.344%
19	19.764	2797	2804	2813	rBV7	20348	42760	1.43%	0.295%
20	20.023	2843	2848	2850	rBV2	26397	39451	1.32%	0.272%
21	20.058	2850	2854	2860	rVB	125928	180838	6.05%	1.248%
22	20.240	2878	2885	2891	rBV	2317937	2989223	100.00%	20.630%
23	20.375	2903	2908	2914	rBV5	12230	29923	1.00%	0.207%
24	20.840	2981	2987	2991	rBV4	15595	32148	1.08%	0.222%
25	21.539	3102	3106	3116	rVB4	81089	157502	5.27%	1.087%
26	21.645	3120	3124	3133	rVB2	57456	112142	3.75%	0.774%
27	21.956	3169	3177	3183	rBV	464488	905778	30.30%	6.251%
28	22.003	3183	3185	3192	rVB2	51022	81777	2.74%	0.564%
29	23.489	3433	3438	3447	rVB8	45433	95306	3.19%	0.658%
30	23.707	3470	3475	3484	rVB	60891	131629	4.40%	0.908%
31	24.294	3570	3575	3576	rBV	30916	38149	1.28%	0.263%
32	24.365	3583	3587	3596	rVB7	35490	78144	2.61%	0.539%
33	25.082	3703	3709	3716	rVB2	22052	60515	2.02%	0.418%
34	25.229	3730	3734	3743	rVB2	33271	91038	3.05%	0.628%
35	25.405	3753	3764	3774	rBV2	279300	854799	28.60%	5.899%

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011323\
Data File : BG056282.D
Acq On : 13 Jan 2023 17:57
Operator : CG/JU
Sample : O1135-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-2

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-BG122722.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

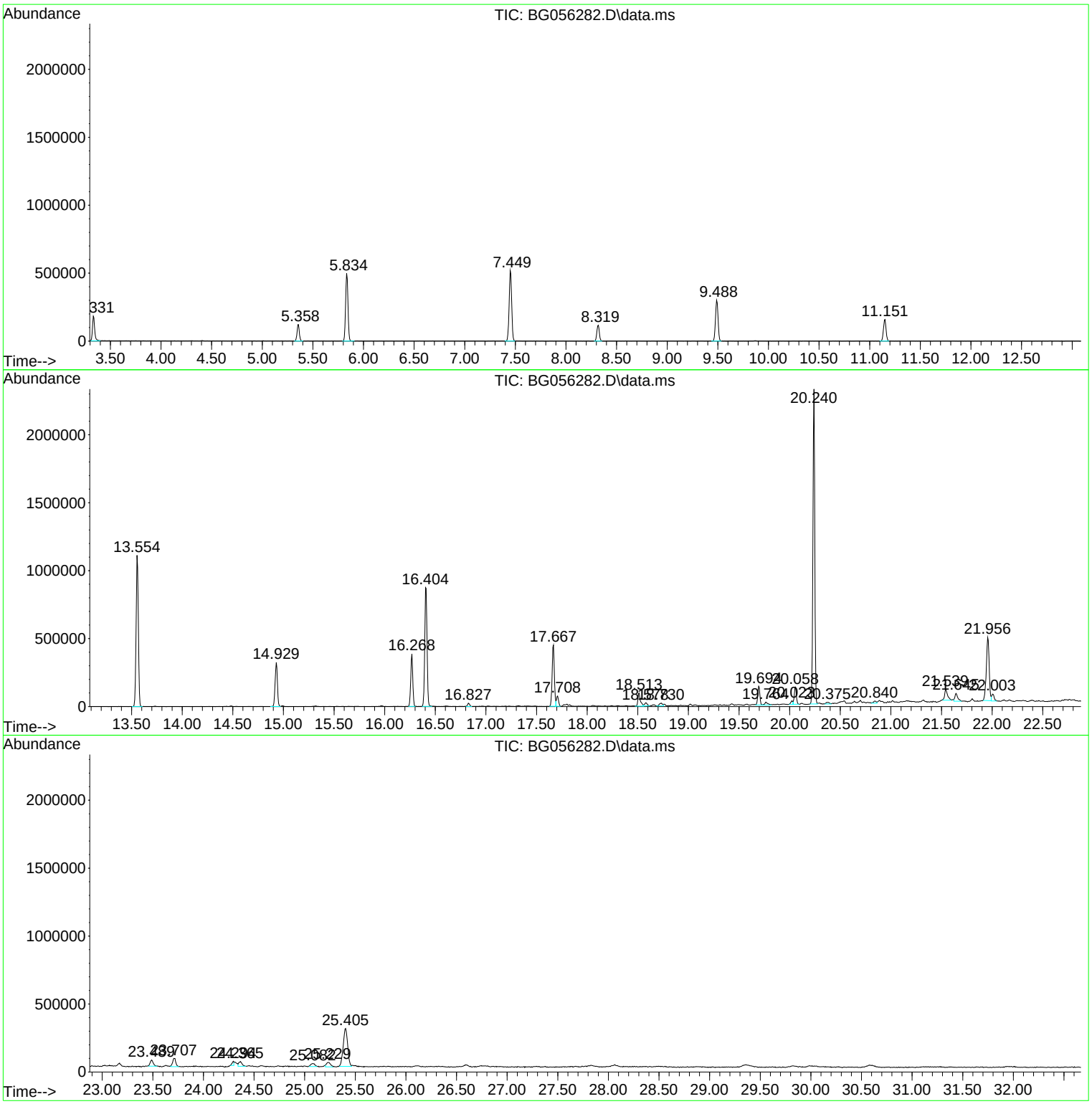
Sum of corrected areas: 14489916

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011323\
Data File : BG056282.D
Acq On : 13 Jan 2023 17:57
Operator : CG/JU
Sample : O1135-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.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\BG011323\
Data File : BG056282.D
Acq On : 13 Jan 2023 17:57
Operator : CG/JU
Sample : O1135-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-2

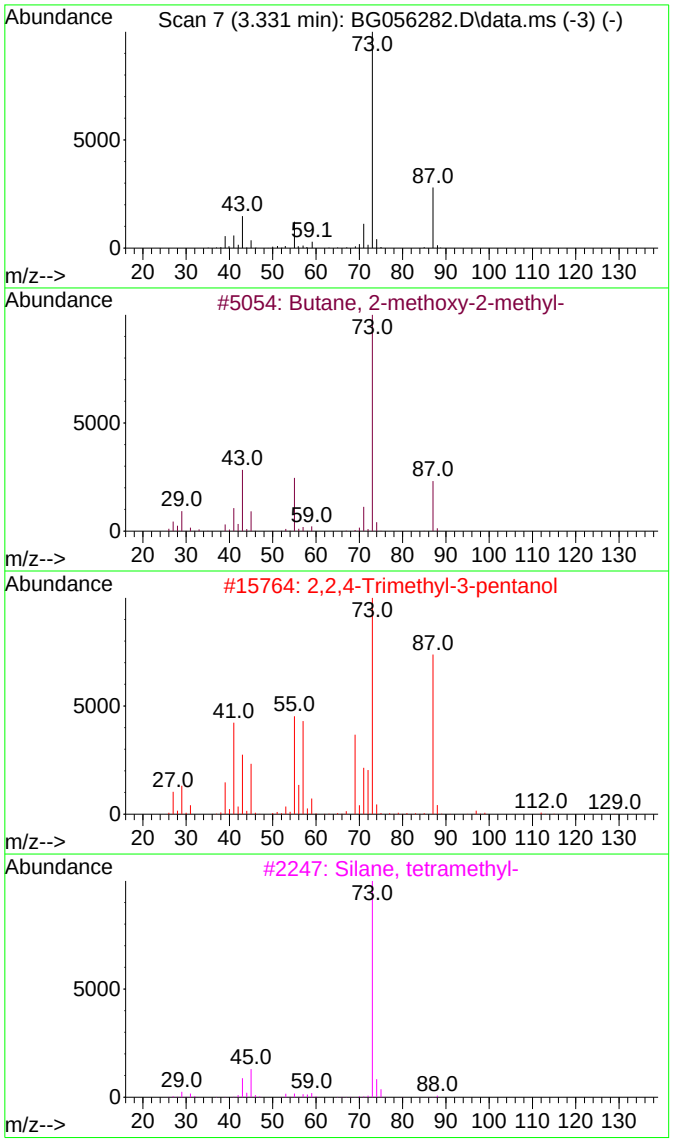
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

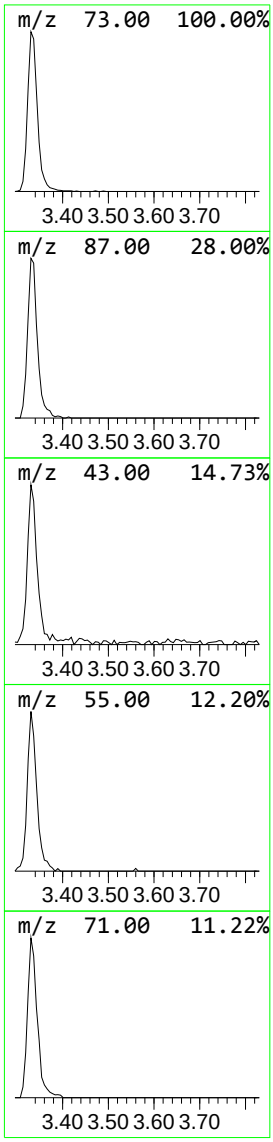
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.331	26.81 ng	267063	1,4-Dichlorobenzene-d4	8.319

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	36
3	Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
4	1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	9
5	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011323\
Data File : BG056282.D
Acq On : 13 Jan 2023 17:57
Operator : CG/JU
Sample : O1135-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-2

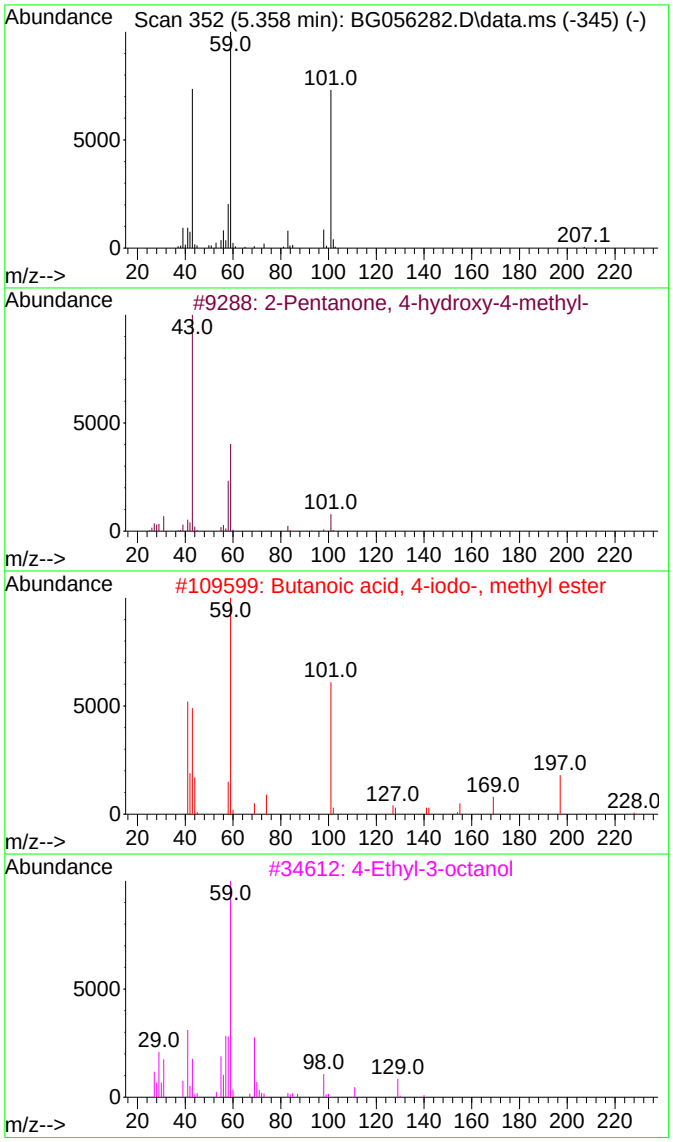
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

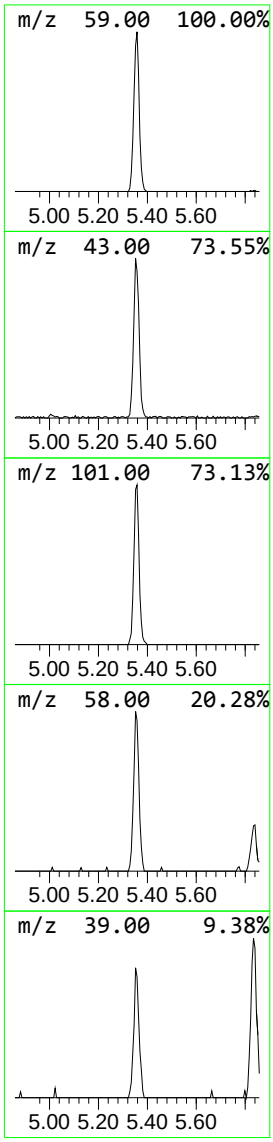
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.358	19.20 ng	191291	1,4-Dichlorobenzene-d4	8.319

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Butanoic acid, 4-iodo-, methyl e...	228	C5H9IO2	014273-85-9	43
3	4-Ethyl-3-octanol	158	C10H22O	019781-26-1	38
4	Succinic acid, hexyl 3-oxobut-2-...	272	C14H24O5	1000349-58-1	27
5	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	22





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011323\
Data File : BG056282.D
Acq On : 13 Jan 2023 17:57
Operator : CG/JU
Sample : O1135-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

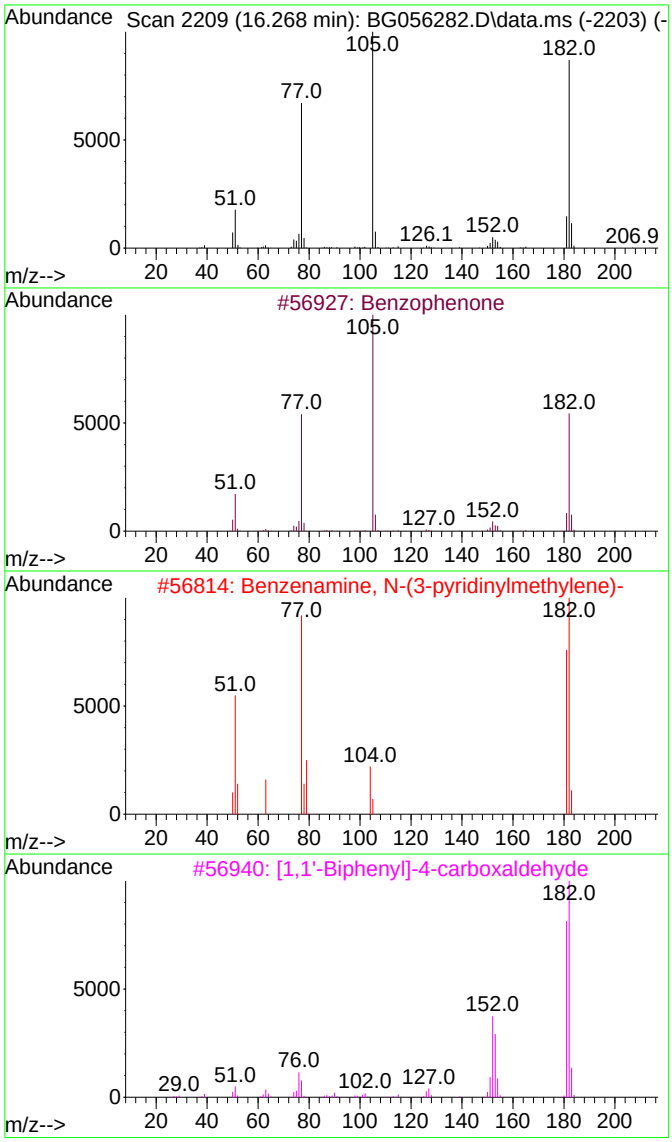
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

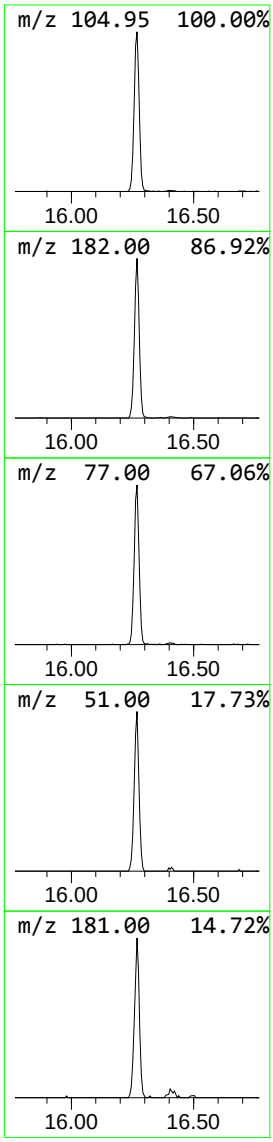
****

Peak Number 3 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.269	21.07 ng	536491	Acenaphthene-d10	14.929

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	95
2	Benzenamine, N-(3-pyridinylmethy...	182	C12H10N2	029722-97-2	53
3	[1,1'-Biphenyl]-4-carboxaldehyde	182	C13H10O	003218-36-8	52
4	3,3'-Dimethylbiphenyl	182	C14H14	000612-75-9	47
5	2,4,6-Trimethoxytoluene	182	C10H14O3	014107-97-2	46





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011323\
Data File : BG056282.D
Acq On : 13 Jan 2023 17:57
Operator : CG/JU
Sample : O1135-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

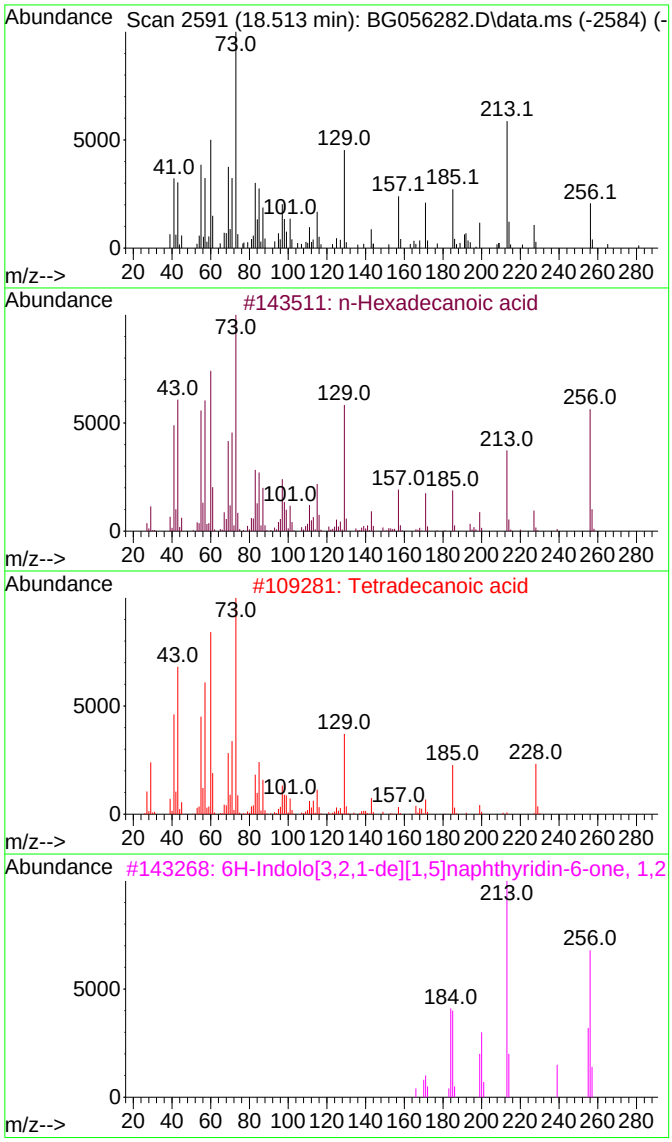
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

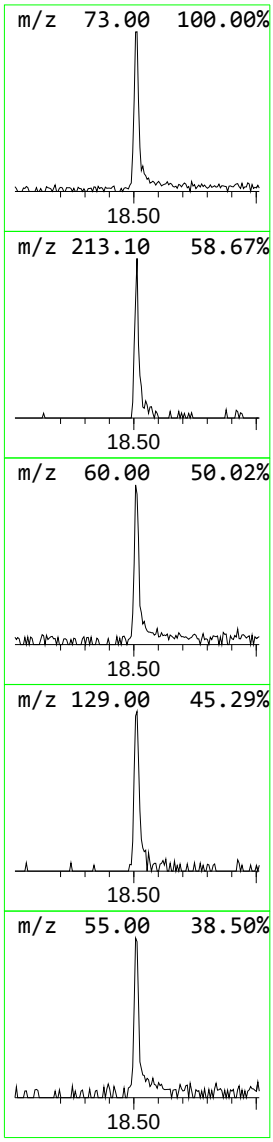
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.513	4.71 ng	164083	Phenanthrene-d10	17.667

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
3	6H-Indolo[3,2,1-de][1,5]naphthyr...	256	C15H16N2O2	050630-67-6	59
4	Tridecanoic acid	214	C13H26O2	000638-53-9	58
5	Dodecanoic acid	200	C12H24O2	000143-07-7	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011323\
Data File : BG056282.D
Acq On : 13 Jan 2023 17:57
Operator : CG/JU
Sample : O1135-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-2

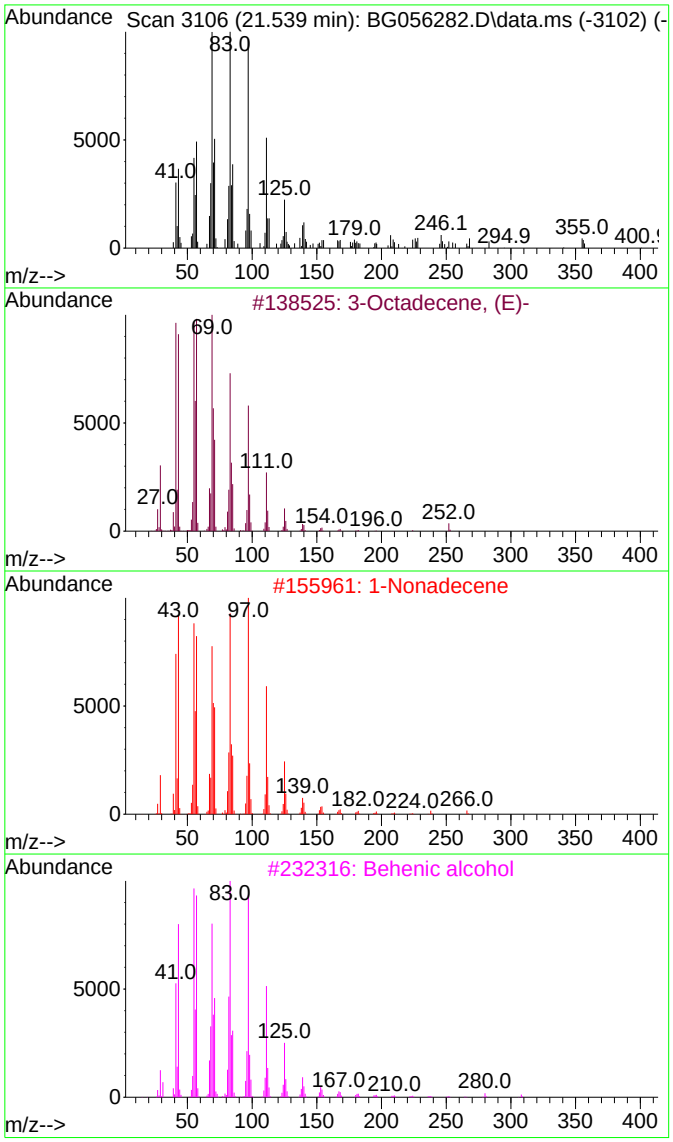
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

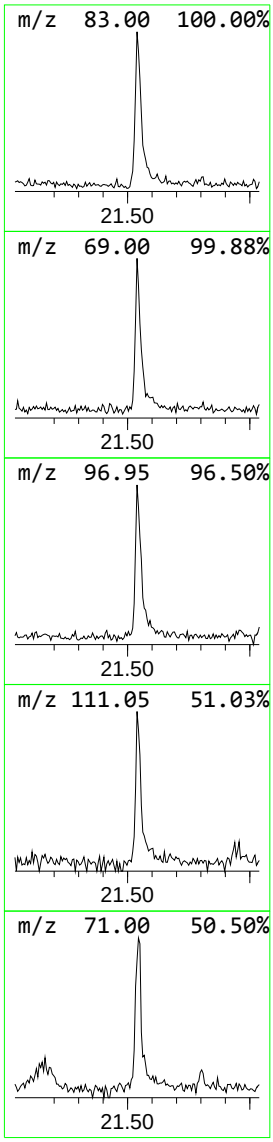
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 3-Octadecene, (E)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.539	3.48 ng	157502	Chrysene-d12	21.956

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Octadecene, (E)-	252	C18H36	007206-19-1	83
2	1-Nonadecene	266	C19H38	018435-45-5	76
3	Behenic alcohol	326	C22H46O	000661-19-8	59
4	1,2-Dodecanediol	202	C12H26O2	001119-87-5	50
5	1-Hexacosanol	382	C26H54O	000506-52-5	45





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011323\
Data File : BG056282.D
Acq On : 13 Jan 2023 17:57
Operator : CG/JU
Sample : O1135-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-2

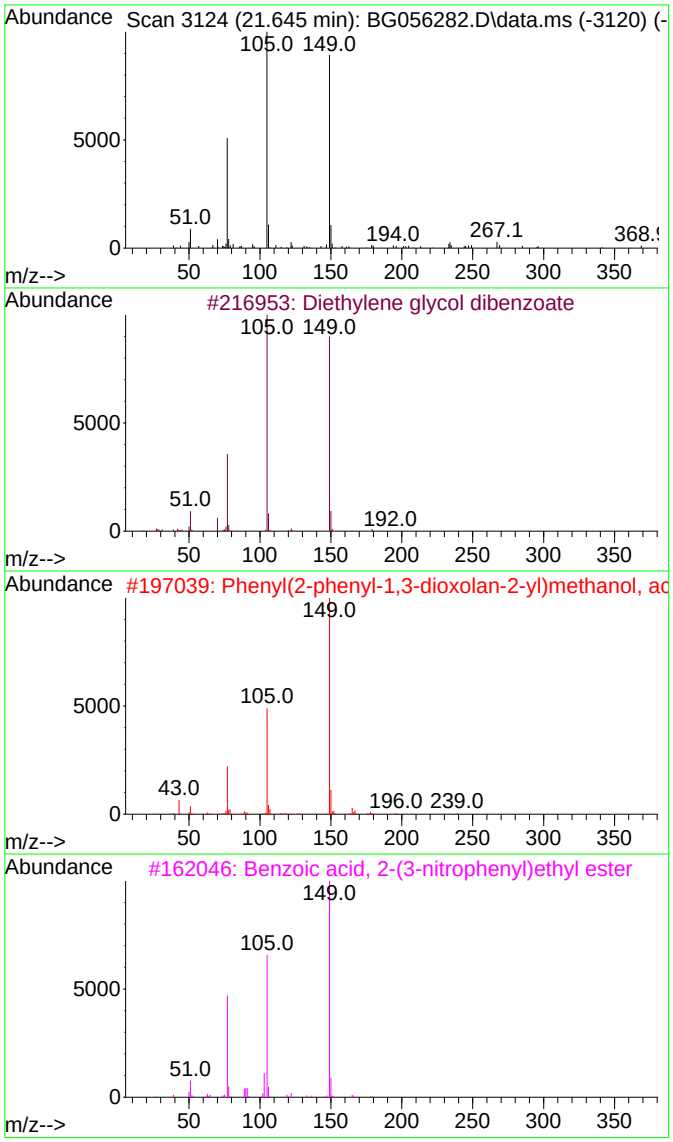
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

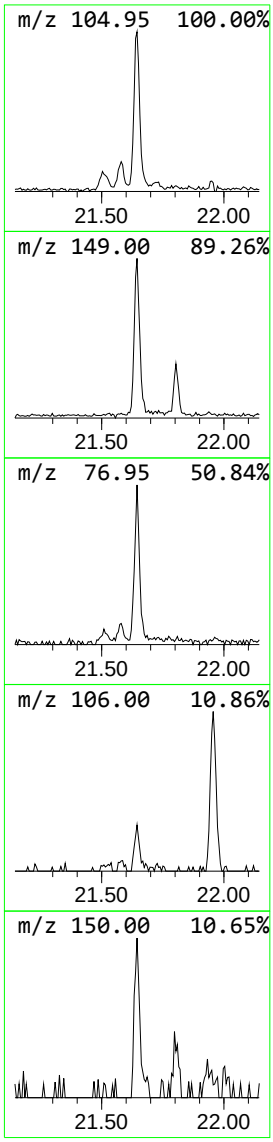
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Diethylene glycol dibenzoate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.645	2.48 ng	112142	Chrysene-d12	21.956

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	78
2	Phenyl(2-phenyl-1,3-dioxolan-2-y...	298	C18H18O4	006963-16-2	78
3	Benzoic acid, 2-(3-nitrophenyl)e...	271	C15H13NO4	1000368-22-4	78
4	Phenyl(2-phenyl-1,3-dioxolan-2-y...	270	C17H18O3	1000507-07-6	78
5	Phthalic acid, heptyl tridec-2-y...	442	C28H42O4	1000315-44-0	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011323\
Data File : BG056282.D
Acq On : 13 Jan 2023 17:57
Operator : CG/JU
Sample : O1135-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-2

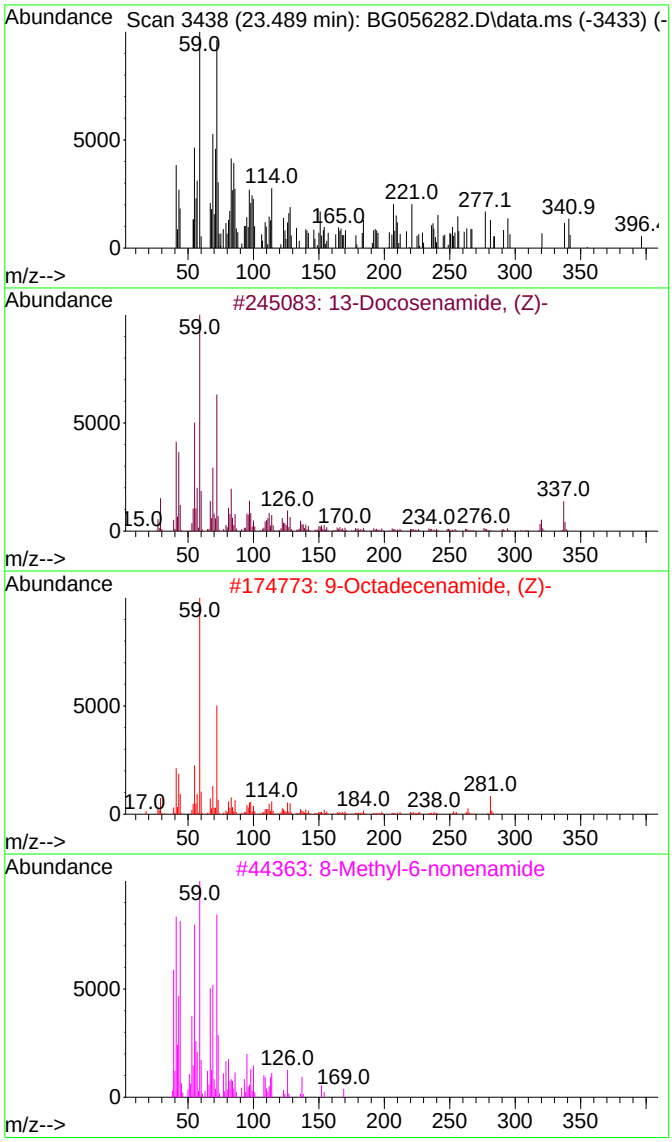
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

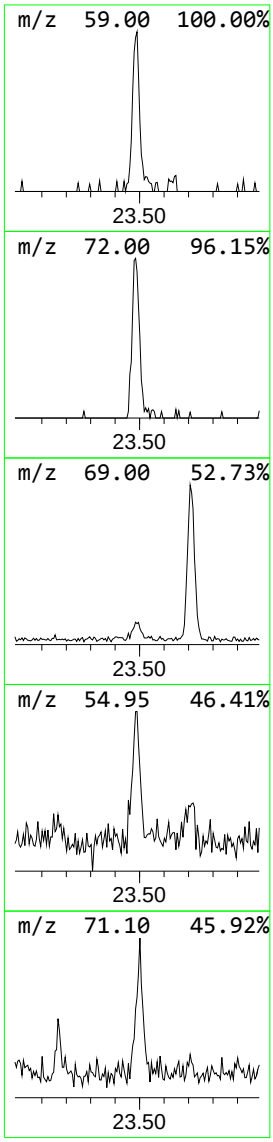
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 13-Docosenamide, (Z)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.489	2.10 ng	95306	Chrysene-d12	21.956

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	58
2	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	52
3	8-Methyl-6-nonenamide	169	C10H19NO	1000293-20-9	49
4	1,1-Dimethyl-1-silacyclobutane	100	C5H12Si	002295-12-7	46
5	Palmitoleamide	253	C16H31NO	106010-22-4	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011323\
Data File : BG056282.D
Acq On : 13 Jan 2023 17:57
Operator : CG/JU
Sample : O1135-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

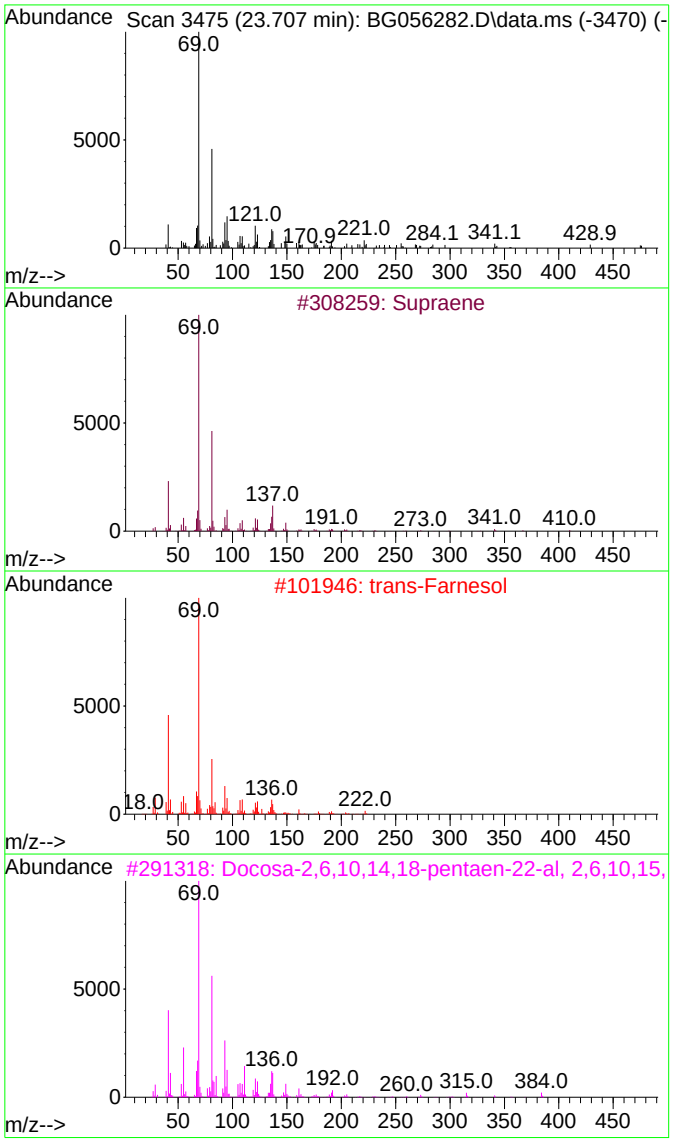
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

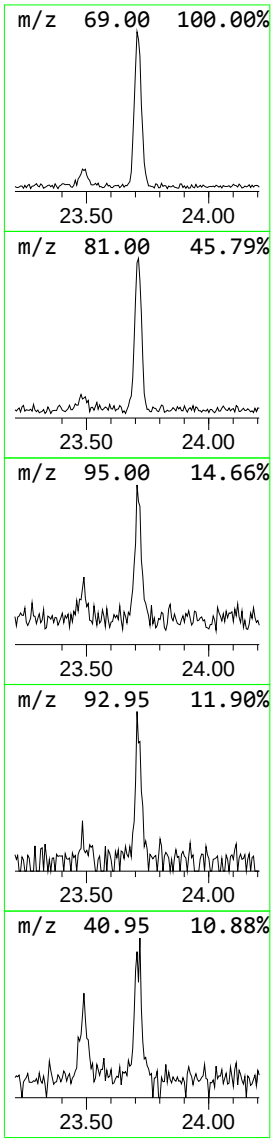
****

Peak Number 8 Supraene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.707	3.08 ng	131629	Perylene-d12	25.399

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	80
2	trans-Farnesol	222	C15H26O	000106-28-5	76
3	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	72
4	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64
5	2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011323\
Data File : BG056282.D
Acq On : 13 Jan 2023 17:57
Operator : CG/JU
Sample : O1135-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.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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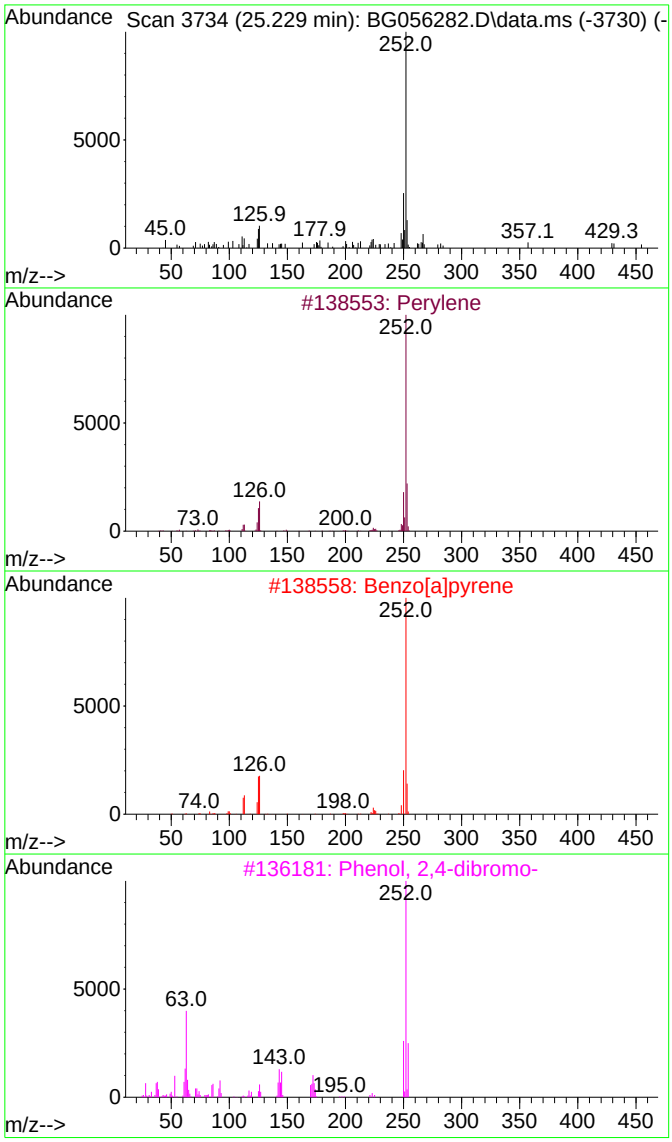
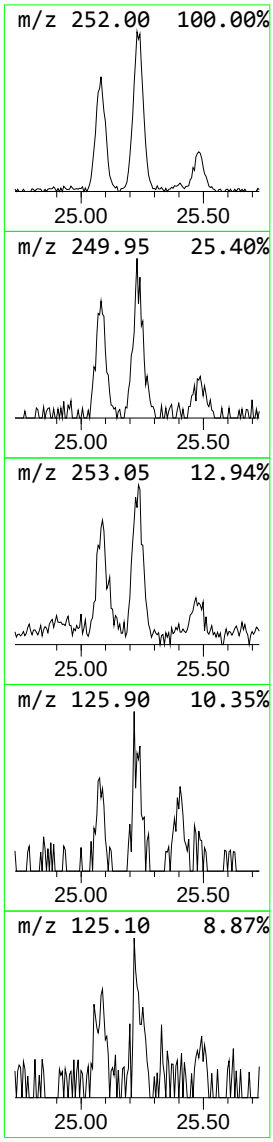
Peak Number 9 Perylene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.229	2.13 ng	91038	Perylene-d12	25.399

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Perylene	252	C20H12	000198-55-0	62
2	Benzo[a]pyrene	252	C20H12	000050-32-8	62
3	Phenol, 2,4-dibromo-	250	C6H4Br2O	000615-58-7	59
4	Benzo[e]pyrene	252	C20H12	000192-97-2	58
5	[1,1'-Biphenyl]-4,4'-diamine, 3,...	252	C12H10Cl2N2	000091-94-1	58





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011323\
Data File : BG056282.D
Acq On : 13 Jan 2023 17:57
Operator : CG/JU
Sample : O1135-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	Internal Standard #	RT	Resp	Conc
Butane, 2-metho...	3.331	26.8	ng	267063	1	8.319	199250	20.0
2-Pentanone, 4-...	5.358	19.2	ng	191291	1	8.319	199250	20.0
Benzophenone	16.269	21.1	ng	536491	3	14.929	509301	20.0
n-Hexadecanoic ...	18.513	4.7	ng	164083	4	17.667	696328	20.0
3-Octadecene, (E)-	21.539	3.5	ng	157502	5	21.956	905778	20.0
Diethylene glyc...	21.645	2.5	ng	112142	5	21.956	905778	20.0
13-Docosenamide...	23.489	2.1	ng	95306	5	21.956	905778	20.0
Supraene	23.707	3.1	ng	131629	6	25.399	854799	20.0
Perylene	25.229	2.1	ng	91038	6	25.399	854799	20.0