LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041824\
Data File : BG060949.D
Acq On : 19 Apr 2024 00:02
Operator : MA/JU
Sample : P2125-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : B-101-SB02

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-BG041724.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG060949.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.157	24	29	44	rVB	109736	173350	3.42%	0.751%
2	3.674	111	117	125	rBV	91297	133152	2.63%	0.577%
3	5.525	425	432	442	rVB	987027	1500526	29.63%	6.498%
4	7.106	692	701	712	rBV	1059123	1791607	35.38%	7.759%
5	7.940	836	843	849	rBV	184767	312262	6.17%	1.352%
6	9.092	1031	1039	1047	rBV	606390	1058630	20.90%	4.584%
7	10.731	1310	1318	1326	rBV	239310	434717	8.58%	1.883%
8	13.193	1729	1737	1744	rBV	1783828	2696526	53.24%	11.677%
9	14.479	1950	1956	1962	rBV	37959	51686	1.02%	0.224%
10	14.568	1962	1971	1977	rVV	451942	701990	13.86%	3.040%
11	16.054	2217	2224	2233	rBV	1819318	2771745	54.73%	12.003%
12	17.311	2430	2438	2448	rBV	673489	1012608	19.99%	4.385%
13	18.216	2587	2592	2602	rBV	376859	538481	10.63%	2.332%
14	19.227	2758	2764	2770	rBV5	39417	56264	1.11%	0.244%
15	19.368	2781	2788	2795	rBV5	27551	67309	1.33%	0.291%
16	19.491	2805	2809	2818	rBV2	126450	253791	5.01%	1.099%
17	19.938	2879	2885	2894	rVB	3830379	5064523	100.00%	21.932%
18	20.085	2906	2910	2914	rVB3	49629	62849	1.24%	0.272%
19	20.220	2928	2933	2937	rBV2	144704	187512	3.70%	0.812%
20	20.496	2976	2980	2985	rVB2	148494	196428	3.88%	0.851%
21	20.555	2985	2990	2997	rBV8	48396	117057	2.31%	0.507%
22	20.655	3003	3007	3012	rBV8	49182	84889	1.68%	0.368%
23	20.813	3028	3034	3041	rVB5	83008	165080	3.26%	0.715%
24	20.972	3057	3061	3066	rVB4	93994	121872	2.41%	0.528%
25	21.036	3069	3072	3077	rBV6	44917	69075	1.36%	0.299%
26	21.248	3103	3108	3118	rBV3	177020	377445	7.45%	1.635%
27	21.330	3119	3122	3129	rVB8	47972	79550	1.57%	0.344%
28	21.571	3157	3163	3167	rBV2	679187	1114313	22.00%	4.826%
29	21.606	3167	3169	3176	rVB3	151266	212243	4.19%	0.919%
30	22.012	3234	3238	3246	rVB10	44481	91313	1.80%	0.395%
31	22.400	3300	3304	3315	rVB4	37386	83079	1.64%	0.360%
32	23.257	3445	3450	3457	rVB	156829	308405	6.09%	1.336%
33	24.691	3684	3694	3706	rBV	448083	1201800	23.73%	5.204%

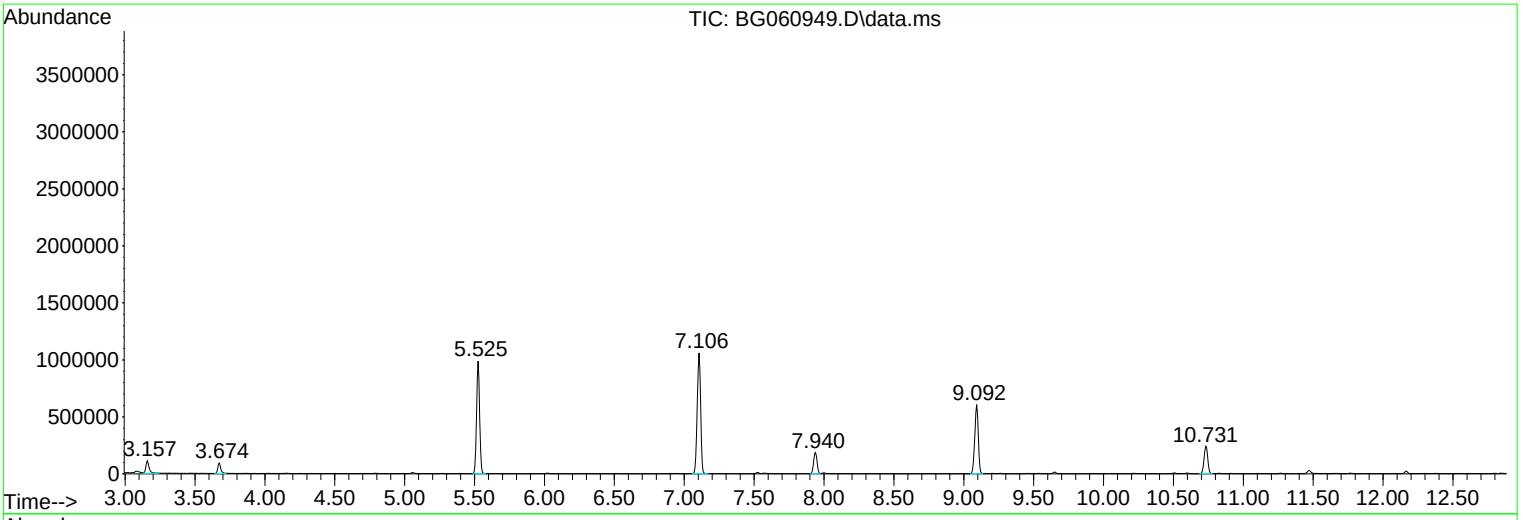
Sum of corrected areas: 23092077

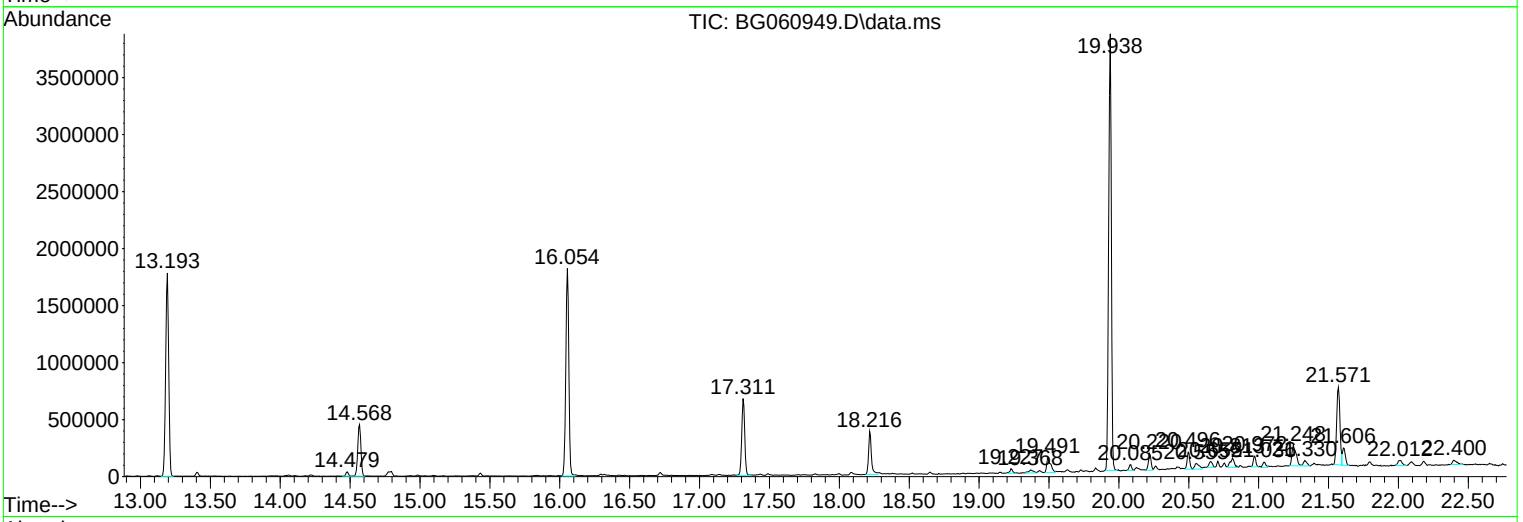
Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041824\
Data File : BG060949.D
Acq On : 19 Apr 2024 00:02
Operator : MA/JU
Sample : P2125-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

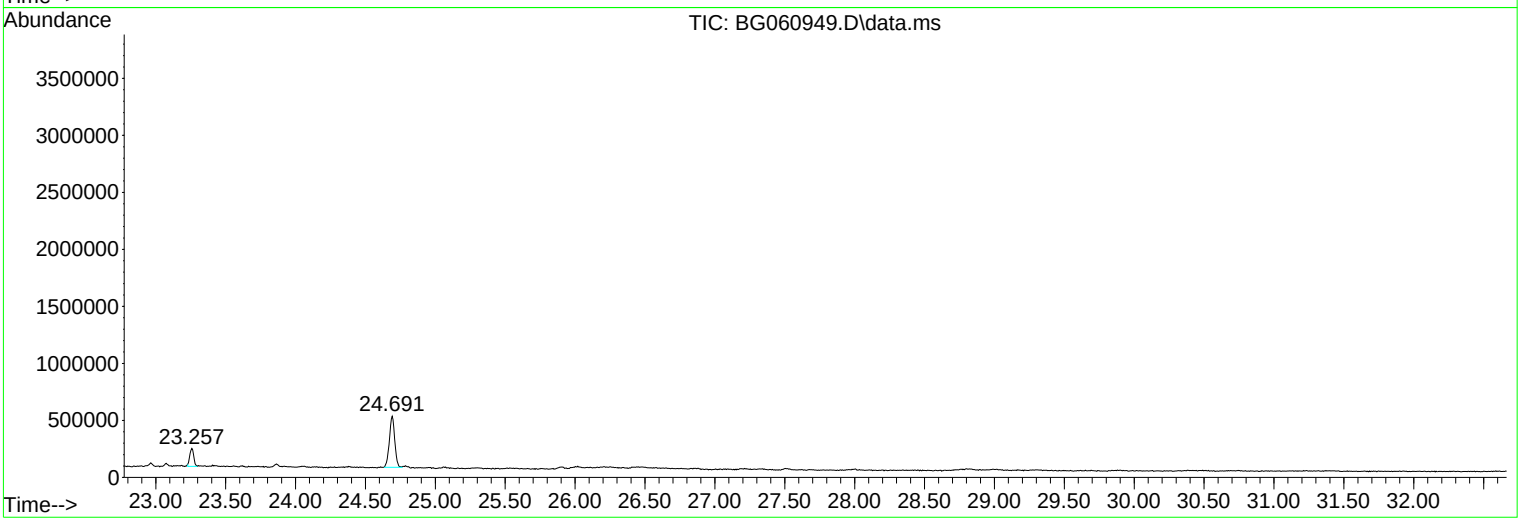
Instrument :
BNA_G
ClientSampleId :
B-101-SB02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG041724.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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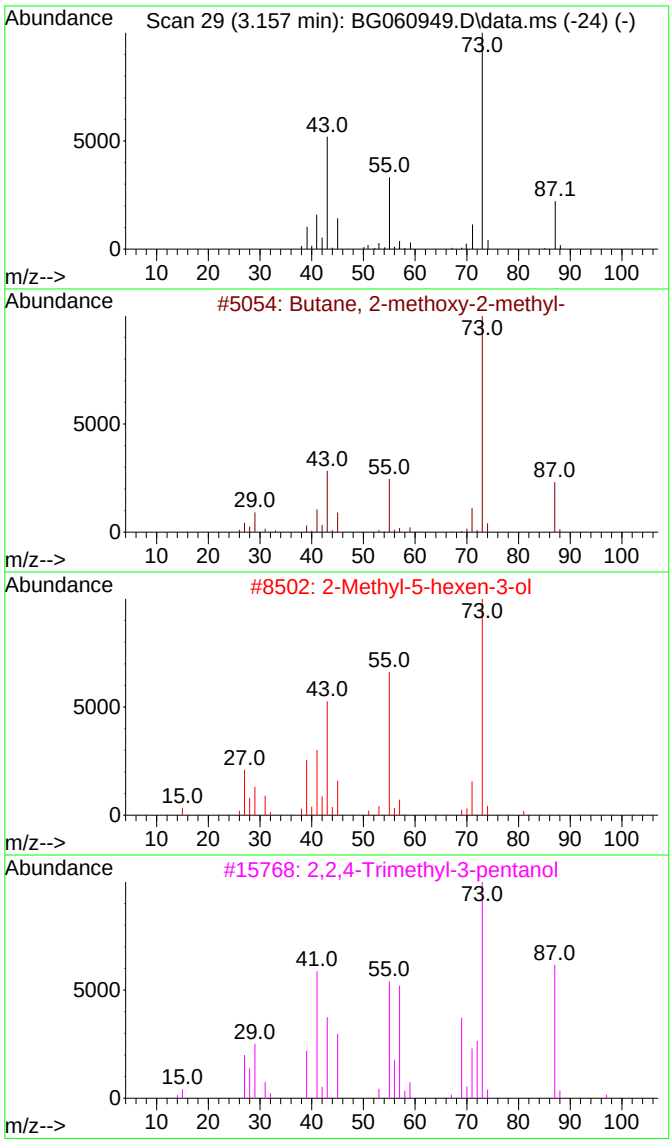
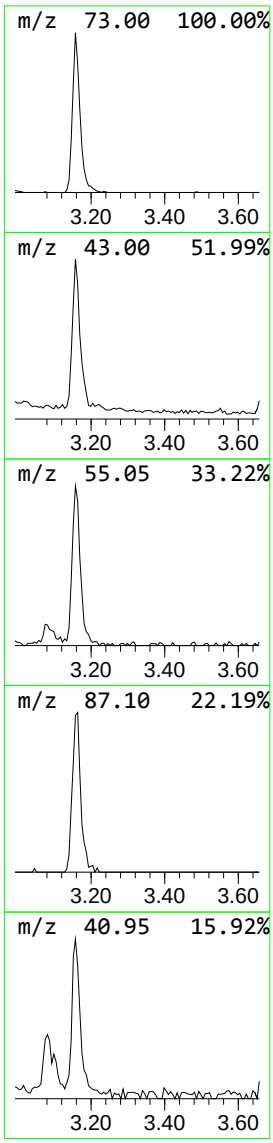
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.157	11.10 ng	173350	1,4-Dichlorobenzene-d4	7.934

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	50
3	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9





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Operator : MA/JU
Sample : P2125-02
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ALS Vial : 13 Sample Multiplier: 1

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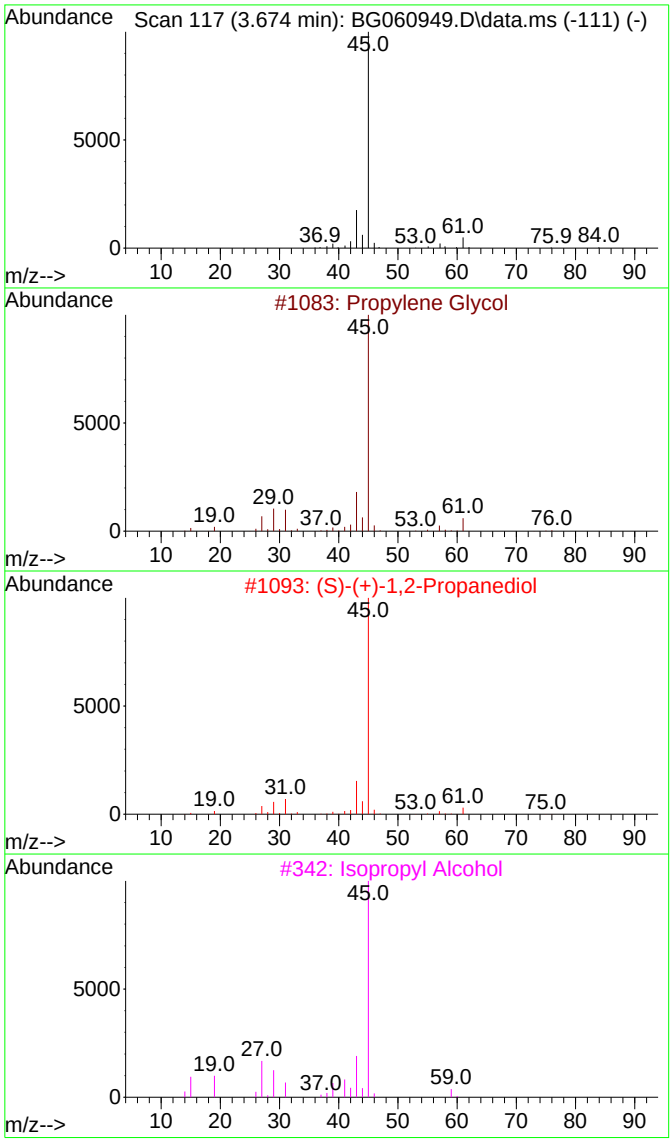
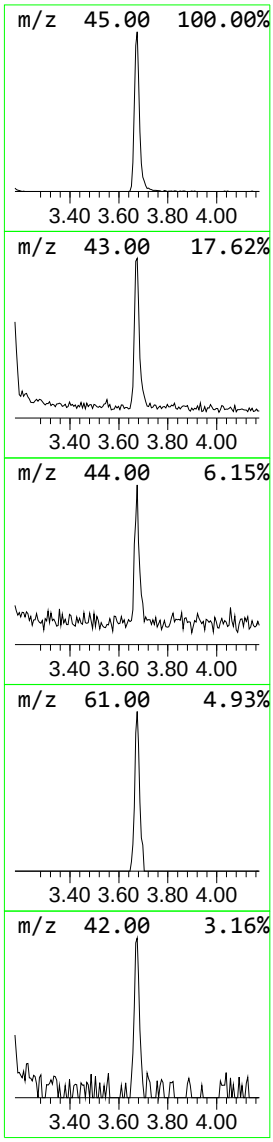
Peak Number 2 Propylene Glycol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.674	8.53 ng	133152	1,4-Dichlorobenzene-d4	7.934

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	78
2	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	56
3	Isopropyl Alcohol	60	C3H8O	000067-63-0	50
4	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	40
5	2-Pentanol	88	C5H12O	006032-29-7	9





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

Instrument :
BNA_G
ClientSampleId :
B-101-SB02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG041724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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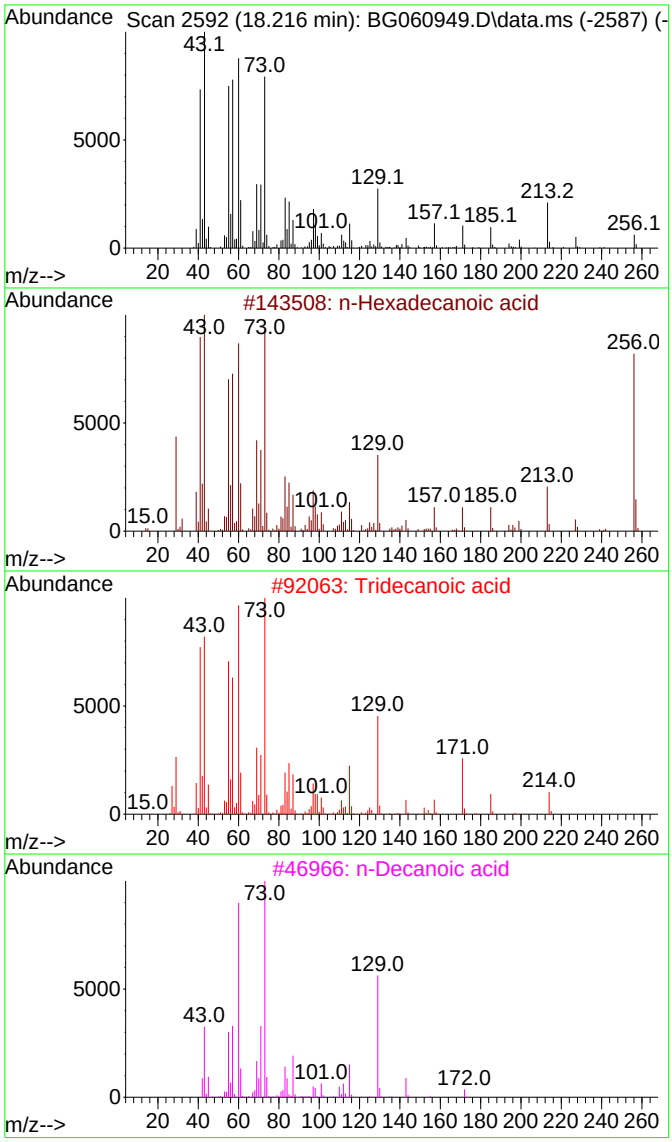
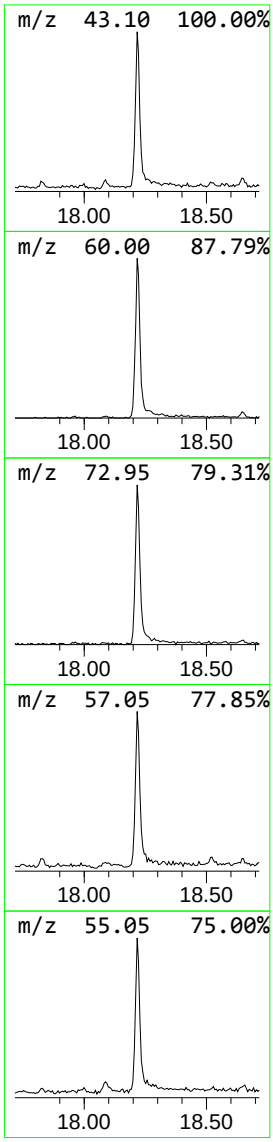
Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.216	10.64 ng	538481	Phenanthrene-d10	17.311

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Tridecanoic acid	214	C13H26O2	000638-53-9	70
3	n-Decanoic acid	172	C10H20O2	000334-48-5	60
4	Octanoic acid	144	C8H16O2	000124-07-2	60
5	Undecanoic acid	186	C11H22O2	000112-37-8	59





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Data File : BG060949.D
Acq On : 19 Apr 2024 00:02
Operator : MA/JU
Sample : P2125-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
B-101-SB02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG041724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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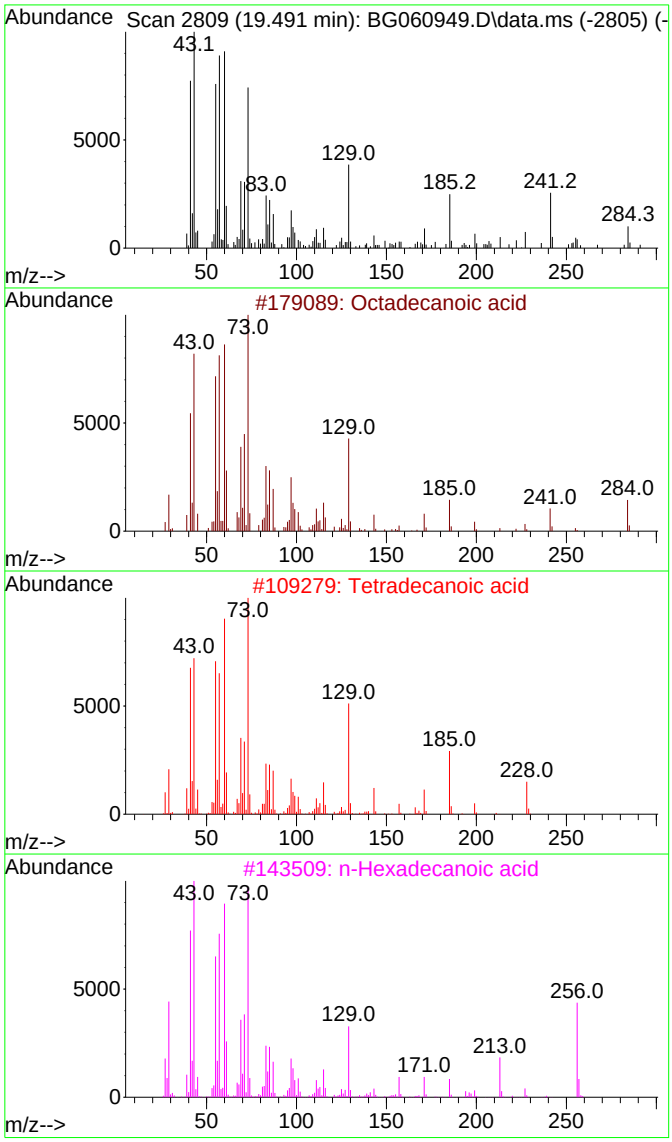
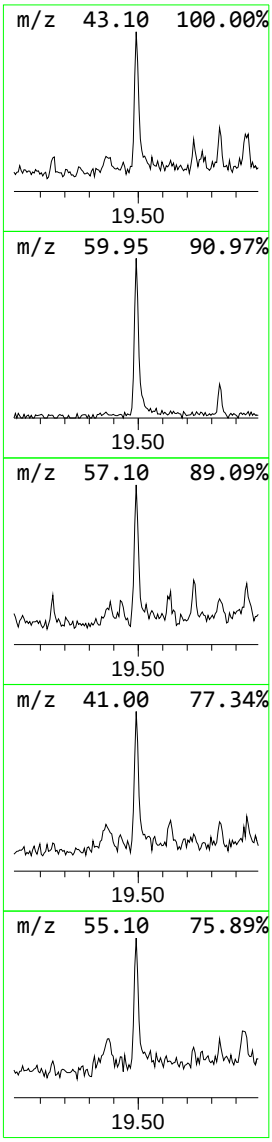
Peak Number 4 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.491	4.56 ng	253791	Chrysene-d12	21.571

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	97
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	86
4	n-Decanoic acid	172	C10H20O2	000334-48-5	64
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	64





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Acq On : 19 Apr 2024 00:02
Operator : MA/JU
Sample : P2125-02
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ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
B-101-SB02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG041724.M
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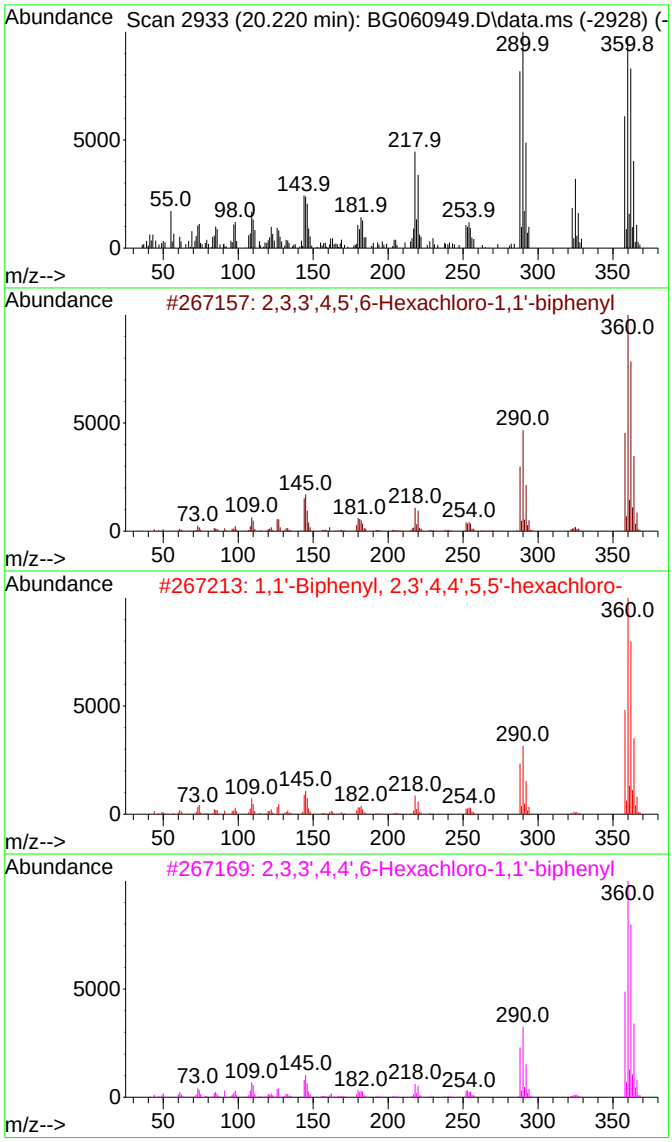
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

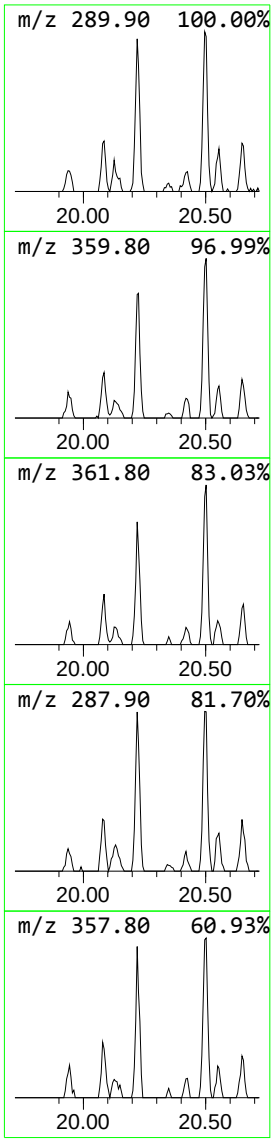
****

Peak Number 5 2,3,3',4,5',6-Hexachloro-1,... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.220	3.37 ng	187512	Chrysene-d12	21.571

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,3,3',4,5',6-Hexachloro-1,1'-bi...	358	C12H4Cl6	074472-43-8	99
2	1,1'-Biphenyl, 2,3',4,4',5,5'-he...	358	C12H4Cl6	052663-72-6	99
3	2,3,3',4,4',6-Hexachloro-1,1'-bi...	358	C12H4Cl6	074472-42-7	99
4	2,2',3,5,6,6'-Hexachloro-1,1'-bi...	358	C12H4Cl6	068194-09-2	99
5	2,3,3',4',5,6-Hexachloro-1,1'-bi...	358	C12H4Cl6	074472-44-9	99





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Instrument :
BNA_G
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG041724.M
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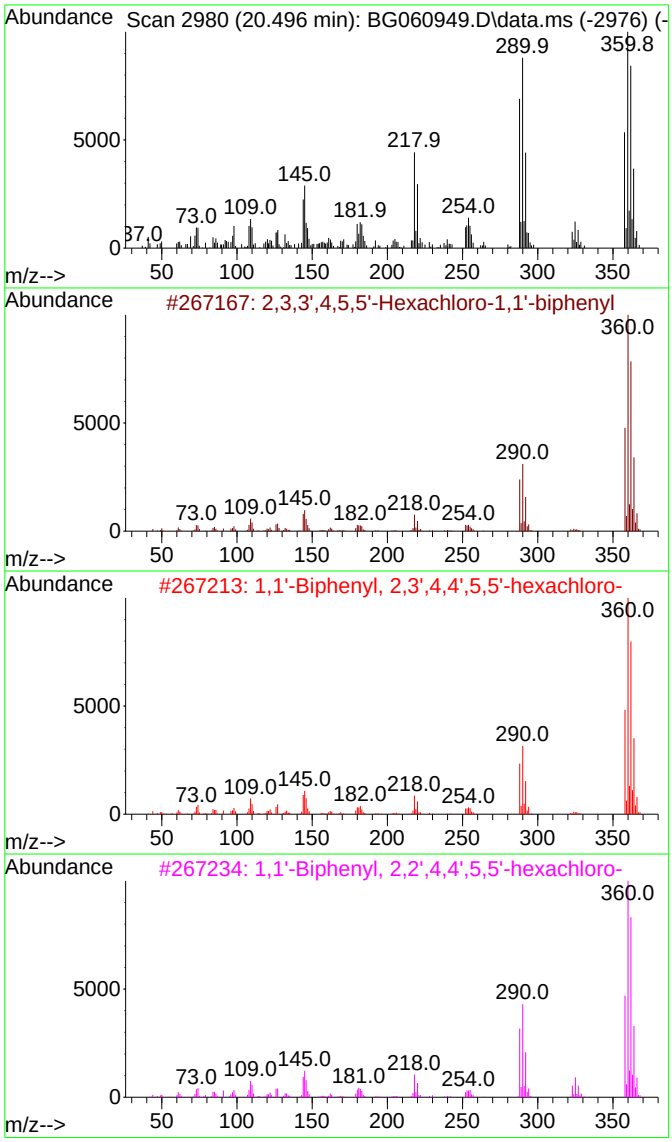
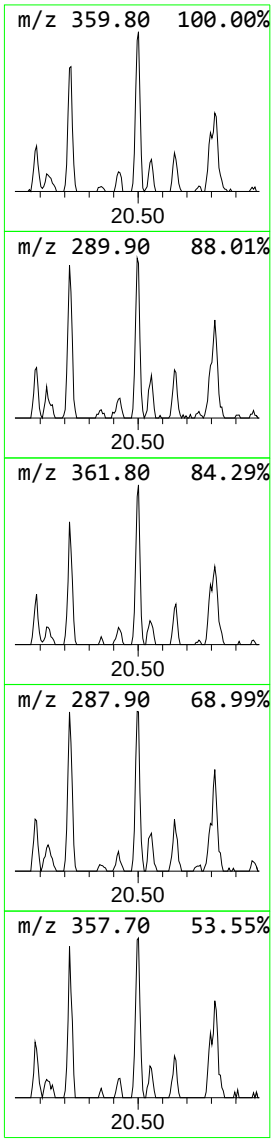
****
Peak Number 6 2,3,3',4,5,5'-Hexachloro-1,... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.496	3.53 ng	196428	Chrysene-d12	21.571

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,3,3',4,5,5'-Hexachloro-1,1'-bi...	358	C12H4Cl6	039635-35-3	99
2	1,1'-Biphenyl, 2,3',4,4',5,5'-he...	358	C12H4Cl6	052663-72-6	99
3	1,1'-Biphenyl, 2,2',4,4',5,5'-he...	358	C12H4Cl6	035065-27-1	99
4	2,3,4,4',5,6-Hexachloro-1,1'-bip...	358	C12H4Cl6	041411-63-6	99
5	2,3,3',4',5',6-Hexachloro-1,1'-b...	358	C12H4Cl6	074472-45-0	98





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Sample : P2125-02
Misc :
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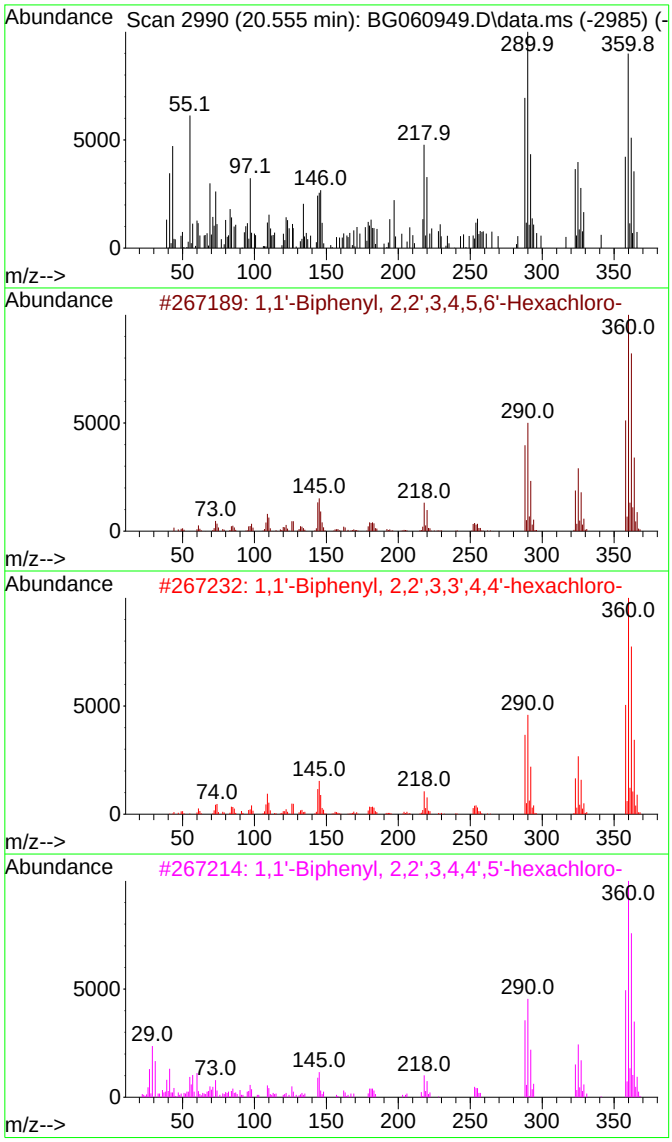
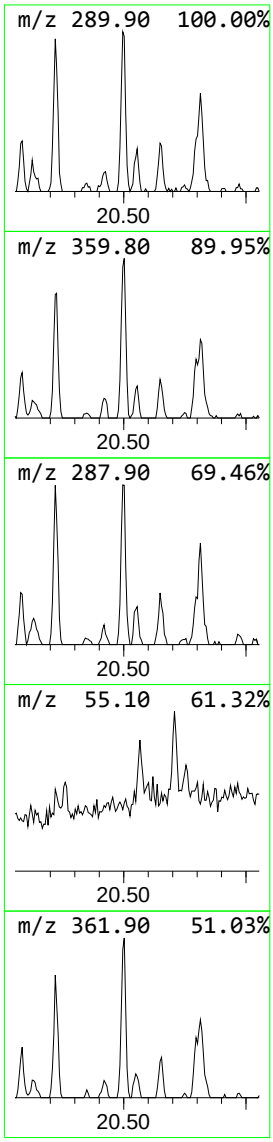
****
Peak Number 7 1,1'-Biphenyl, 2,2',3,4,5,6... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.555	2.10 ng	117057	Chrysene-d12	21.571

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1'-Biphenyl, 2,2',3,4,5,6'-Hex...	358	C12H4Cl6	068194-15-0	99
2	1,1'-Biphenyl, 2,2',3,3',4,4'-he...	358	C12H4Cl6	038380-07-3	99
3	1,1'-Biphenyl, 2,2',3,4,4',5'-he...	358	C12H4Cl6	035065-28-2	99
4	2,2',3,3',5,6-Hexachloro-1,1'-bi...	358	C12H4Cl6	052704-70-8	99
5	1,1'-Biphenyl, 2,2',3,5,5',6-hex...	358	C12H4Cl6	052663-63-5	99





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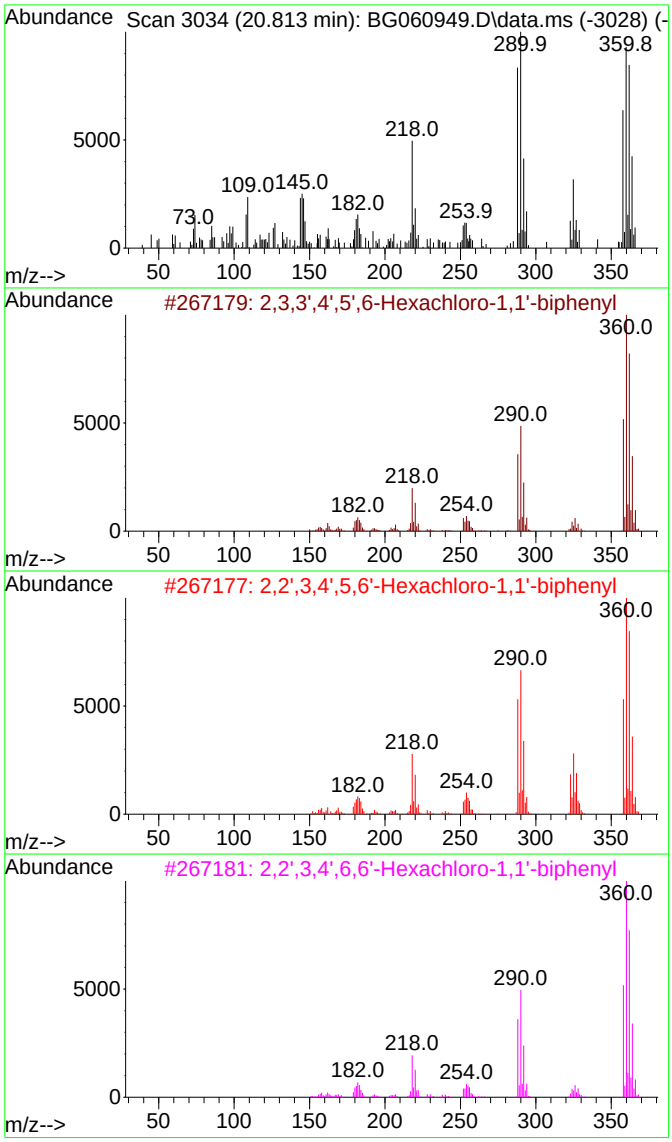
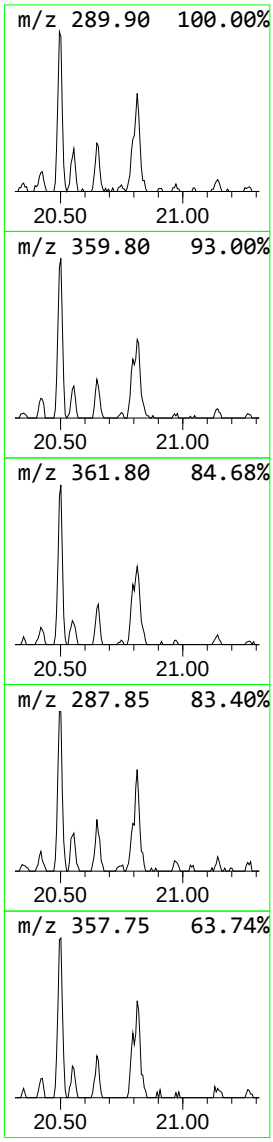
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 2,3,3',4',5',6-Hexachloro-1... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.813	2.96 ng	165080	Chrysene-d12	21.571

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,3,3',4',5',6-Hexachloro-1,1'-b...	358	C12H4Cl6	074472-45-0	99
2	2,2',3,4',5,6'-Hexachloro-1,1'-b...	358	C12H4Cl6	074472-41-6	98
3	2,2',3,4',6,6'-Hexachloro-1,1'-b...	358	C12H4Cl6	068194-08-1	98
4	2,2',3,5,6,6'-Hexachloro-1,1'-bi...	358	C12H4Cl6	068194-09-2	98
5	2,3',4,4',5',6-Hexachloro-1,1'-b...	358	C12H4Cl6	059291-65-5	97





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B-101-SB02

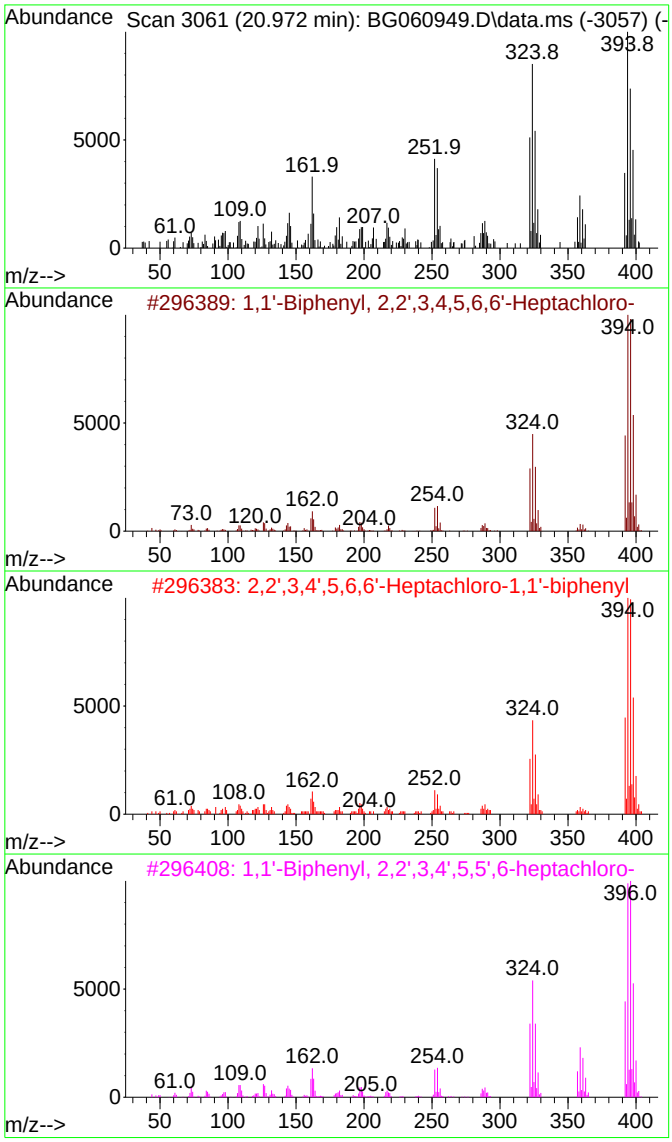
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG041724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

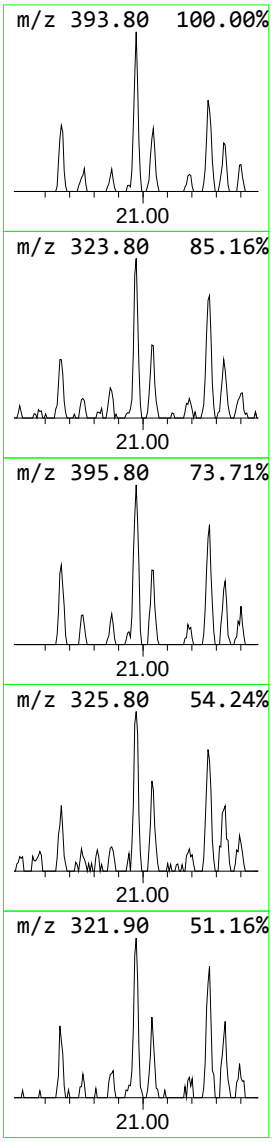
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 1,1'-Biphenyl, 2,2',3,4,5,6... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.972	2.19 ng	121872	Chrysene-d12	21.571

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1'-Biphenyl, 2,2',3,4,5,6,6'-H...	392	C12H3Cl7	074472-49-4	99
2	2,2',3,4',5,6,6'-Heptachloro-1,1...	392	C12H3Cl7	074487-85-7	99
3	1,1'-Biphenyl, 2,2',3,4',5,5',6-...	392	C12H3Cl7	052663-68-0	99
4	1,1'-Biphenyl, 2,2',3,4,4',5,5'-...	392	C12H3Cl7	035065-29-3	99
5	1,1'-Biphenyl, 2,3,3',4,4',5,6-H...	392	C12H3Cl7	041411-64-7	99





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041824\
Data File : BG060949.D
Acq On : 19 Apr 2024 00:02
Operator : MA/JU
Sample : P2125-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
B-101-SB02

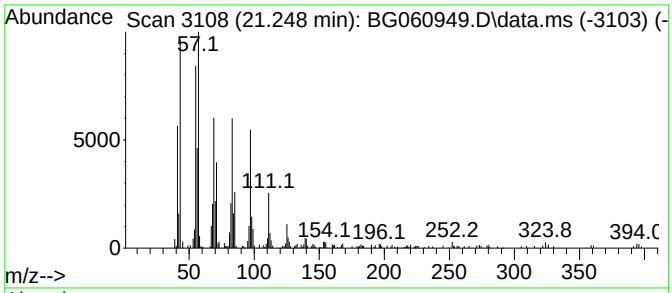
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG041724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

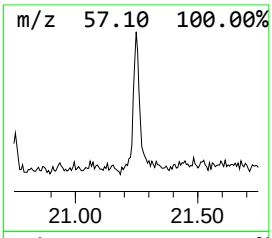
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

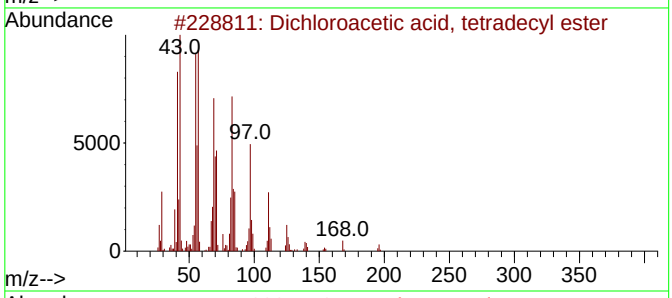
****
Peak Number 10 Dichloroacetic acid, tetrad... Concentration Rank 4

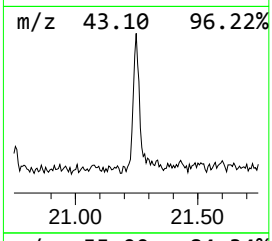
R.T.	EstConc	Area	Relative to ISTD	R.T.
21.248	6.77 ng	377445	Chrysene-d12	21.571

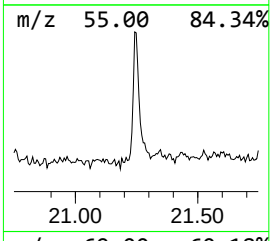
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dichloroacetic acid, tetradecyl ...	324	C16H30Cl2O2	083005-02-1	91
2	13-Tetradecen-1-ol acetate	254	C16H30O2	056221-91-1	90
3	1-Octadecene	252	C18H36	000112-88-9	90
4	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	90
5	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	90

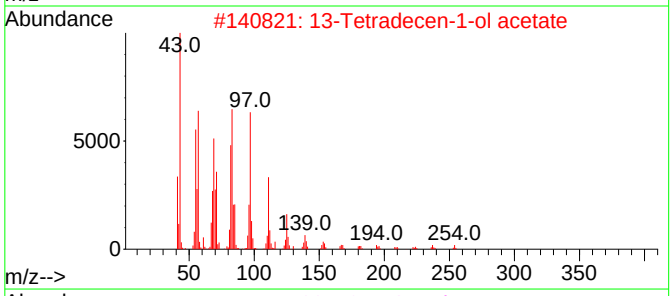


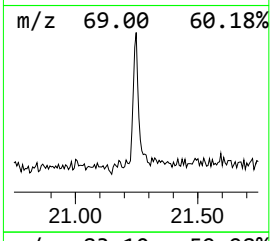


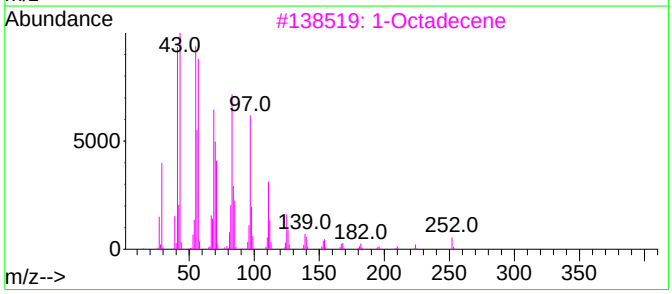


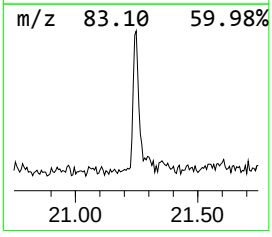












Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041824\
Data File : BG060949.D
Acq On : 19 Apr 2024 00:02
Operator : MA/JU
Sample : P2125-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
B-101-SB02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG041724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

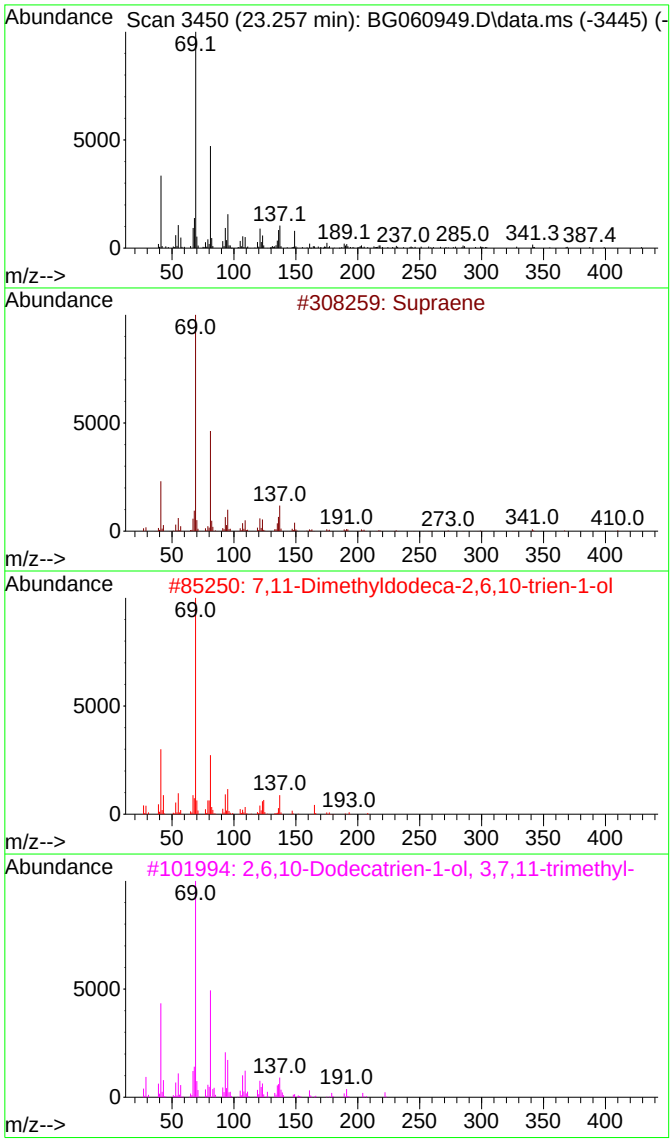
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

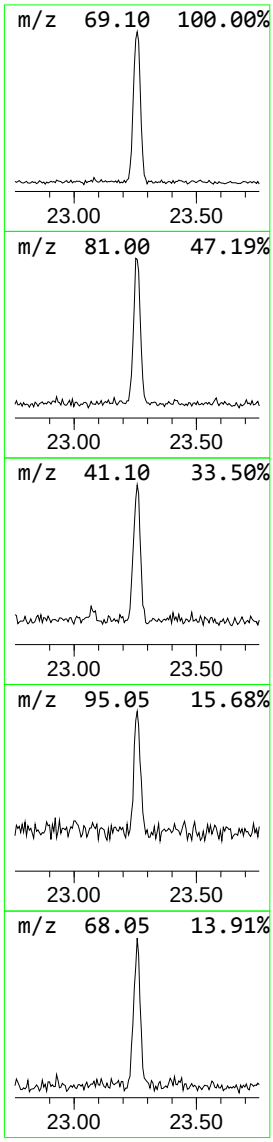
****

Peak Number 11 Supraene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.257	5.13 ng	308405	Perylene-d12	24.691

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	87
2	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64
3	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	64
4	2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	64
5	trans-Farnesol	222	C15H26O	000106-28-5	59





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041824\
Data File : BG060949.D
Acq On : 19 Apr 2024 00:02
Operator : MA/JU
Sample : P2125-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
B-101-SB02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG041724.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...	3.157	11.1	ng	173350	1	7.934	312262	20.0
Propylene Glycol	3.674	8.5	ng	133152	1	7.934	312262	20.0
n-Hexadecanoic ...	18.216	10.6	ng	538481	4	17.311	1012610	20.0
Octadecanoic acid	19.491	4.6	ng	253791	5	21.571	1114310	20.0
2,3,3',4,5',6-H...	20.220	3.4	ng	187512	5	21.571	1114310	20.0
2,3,3',4,5,5'-H...	20.496	3.5	ng	196428	5	21.571	1114310	20.0
1,1'-Biphenyl, ...	20.555	2.1	ng	117057	5	21.571	1114310	20.0
2,3,3',4',5',6-...	20.813	3.0	ng	165080	5	21.571	1114310	20.0
1,1'-Biphenyl, ...	20.972	2.2	ng	121872	5	21.571	1114310	20.0
Dichloroacetic ...	21.248	6.8	ng	377445	5	21.571	1114310	20.0
Supraene	23.257	5.1	ng	308405	6	24.691	1201800	20.0