

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062223\
 Data File : BG057805.D
 Acq On : 22 Jun 2023 11:39
 Operator : CG/JU
 Sample : 03290-02
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SB-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-BG061923.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG057805.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.024	323	329	337	rVB	245001	356532	16.15%	3.149%
2	5.488	402	408	418	rBV	513526	806193	36.51%	7.121%
3	7.080	670	679	688	rBV	557760	927598	42.01%	8.193%
4	7.921	816	822	828	rBV	107230	173927	7.88%	1.536%
5	9.078	1011	1019	1030	rVB	323422	551848	24.99%	4.874%
6	10.723	1292	1299	1307	rBV	158708	274843	12.45%	2.428%
7	13.179	1710	1717	1726	rVB	860949	1300865	58.91%	11.490%
8	14.554	1943	1951	1959	rBV	286729	427780	19.37%	3.778%
9	15.911	2176	2182	2187	rVB	56586	81919	3.71%	0.724%
10	16.041	2197	2204	2214	rBV	796464	1173216	53.13%	10.362%
11	17.298	2411	2418	2423	rBV	421507	599203	27.14%	5.292%
12	18.191	2564	2570	2579	rBV	176495	281616	12.75%	2.487%
13	19.043	2710	2715	2721	rBV2	15997	24572	1.11%	0.217%
14	19.348	2760	2767	2774	rBV	42958	77540	3.51%	0.685%
15	19.460	2782	2786	2798	rBV	61642	104507	4.73%	0.923%
16	19.713	2819	2829	2835	rBV	34164	67603	3.06%	0.597%
17	19.912	2857	2863	2869	rBV	1614321	2208131	100.00%	19.503%
18	21.205	3078	3083	3092	rVB2	148724	221648	10.04%	1.958%
19	21.281	3093	3096	3101	rVB	35722	50015	2.27%	0.442%
20	21.546	3134	3141	3147	rBV	402078	686430	31.09%	6.063%
21	21.751	3171	3176	3181	rBV2	25488	43509	1.97%	0.384%
22	22.351	3274	3278	3285	rVB3	24311	44935	2.03%	0.397%
23	23.021	3389	3392	3398	rVB4	12945	22469	1.02%	0.198%
24	24.701	3668	3678	3694	rVB	253713	750275	33.98%	6.627%
25	25.970	3889	3894	3902	rVB5	27453	64880	2.94%	0.573%

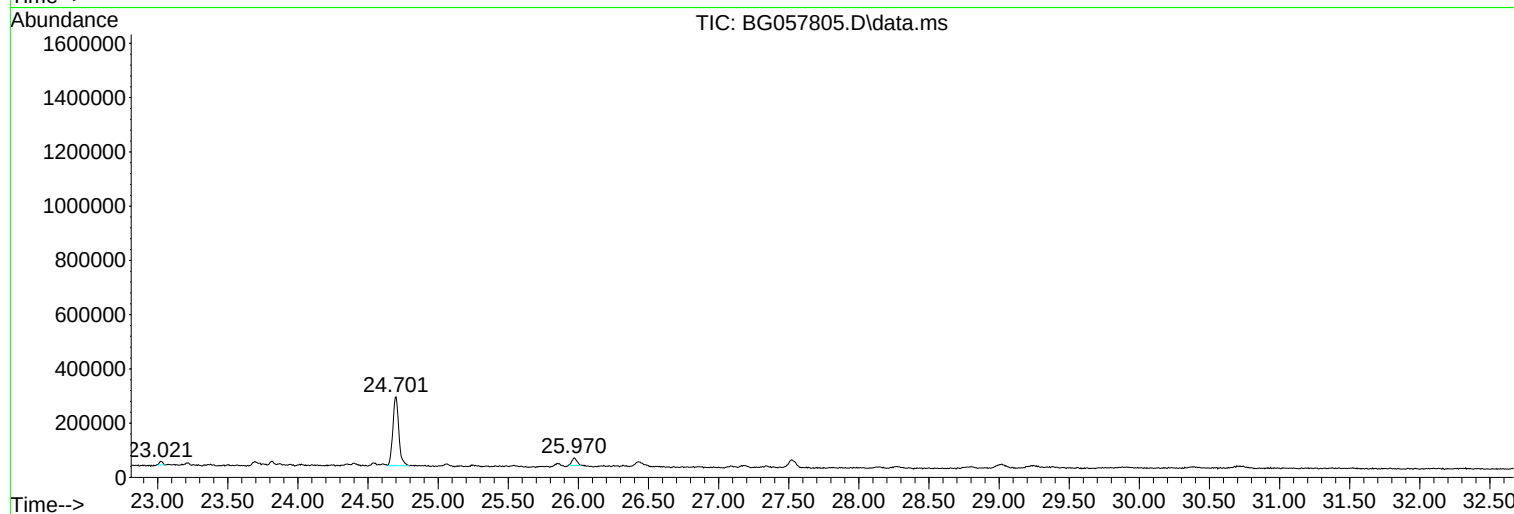
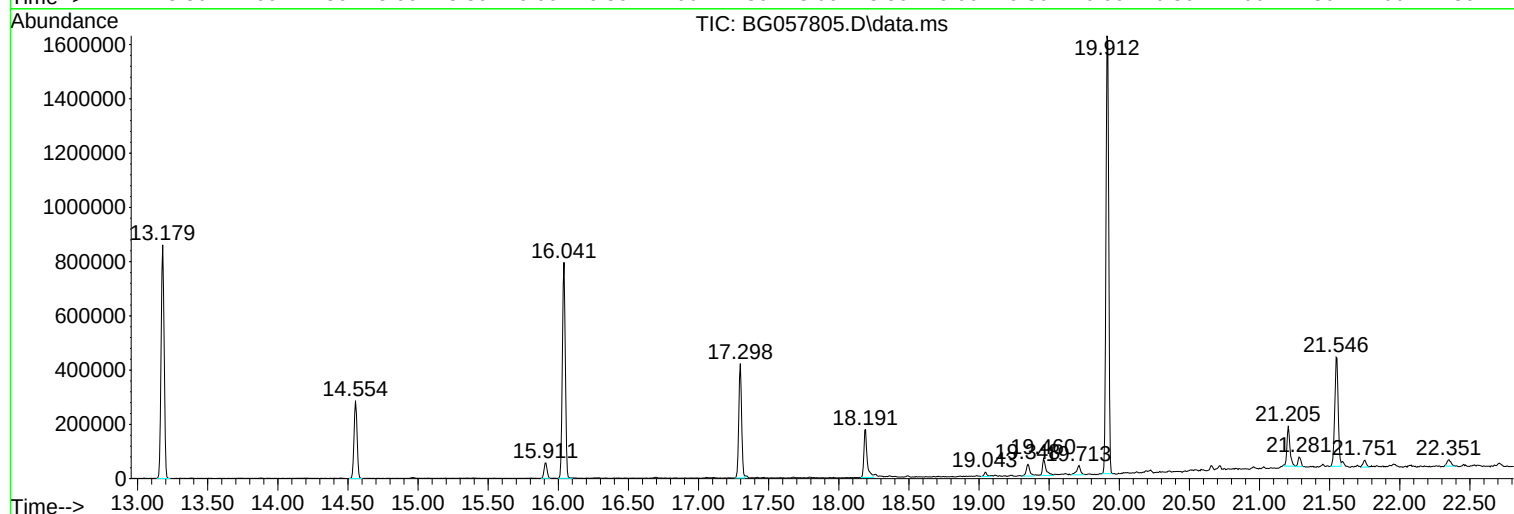
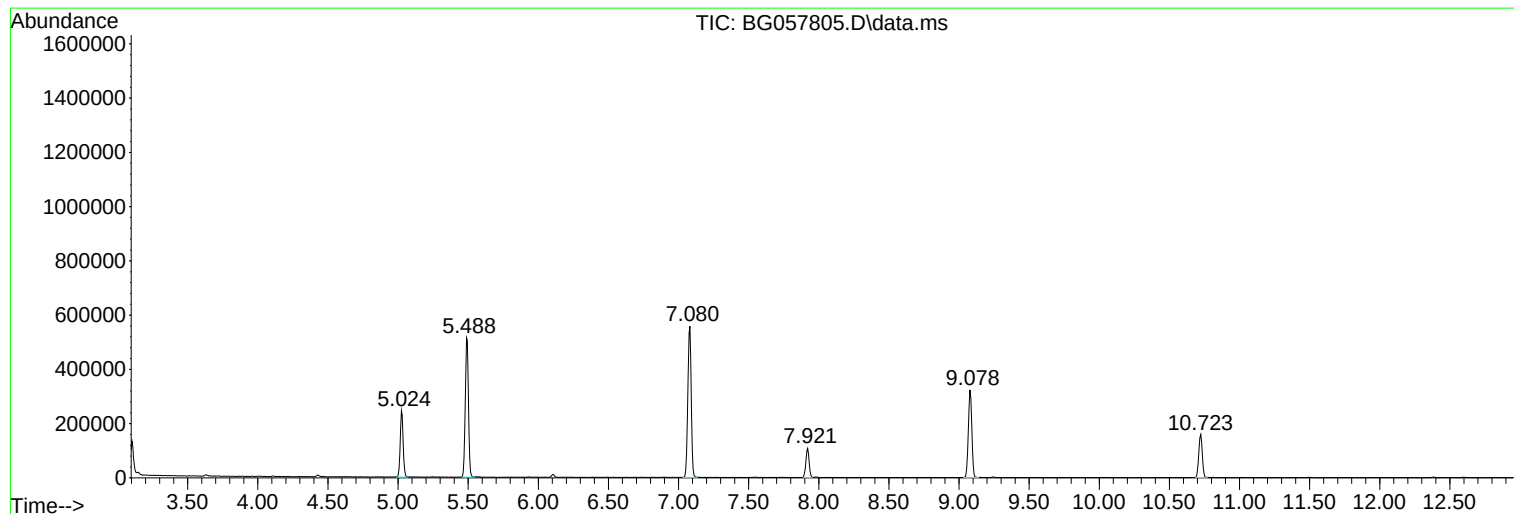
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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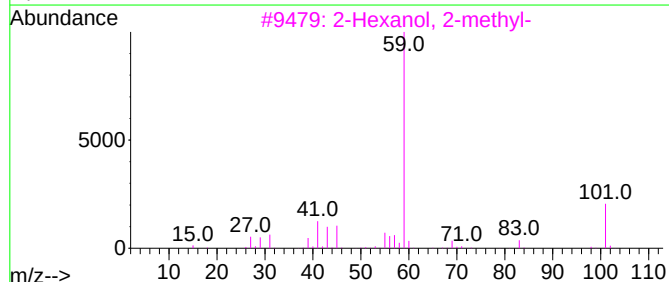
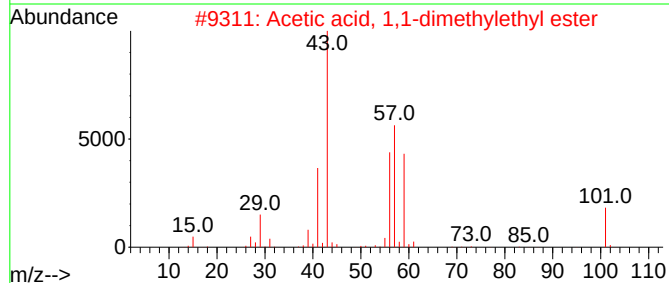
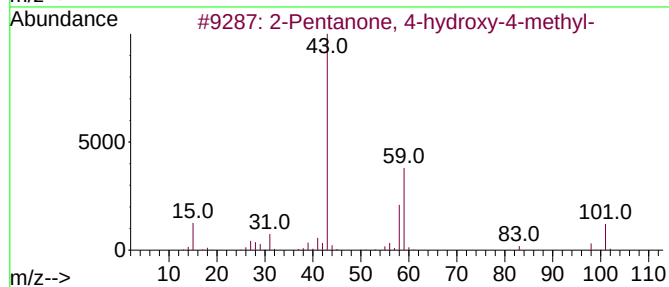
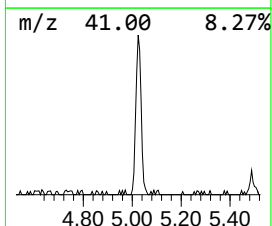
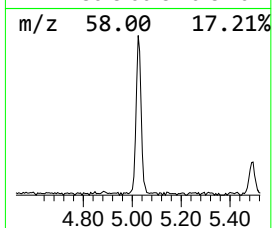
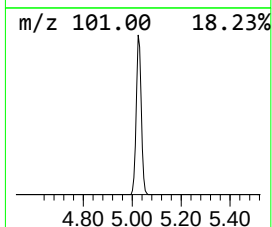
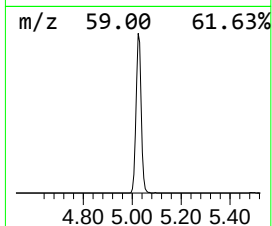
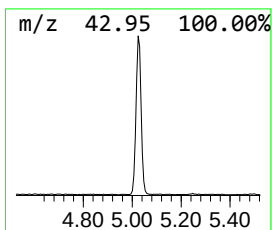
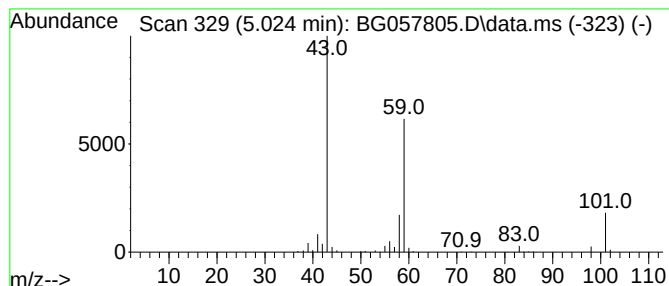
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.024	41.00 ng	356532	1,4-Dichlorobenzene-d4	7.921

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59		
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39		
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	10		



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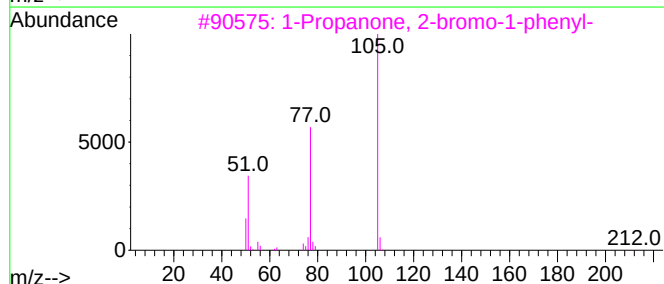
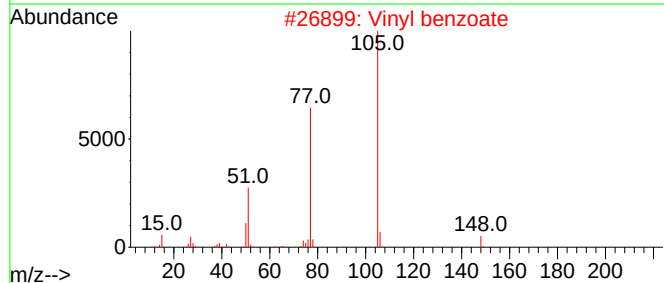
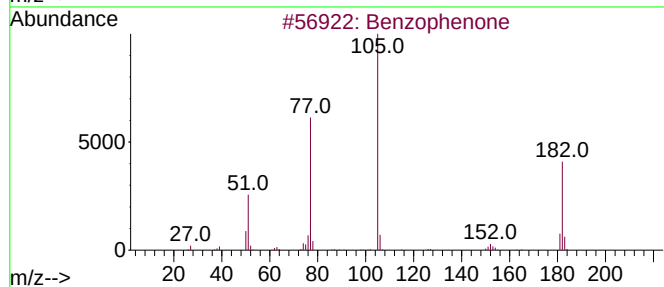
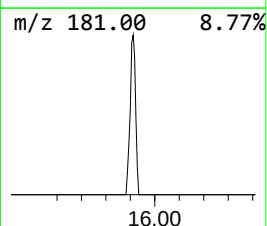
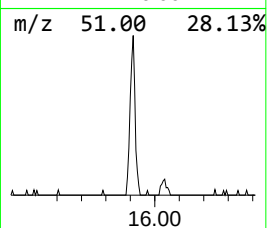
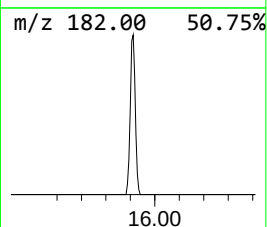
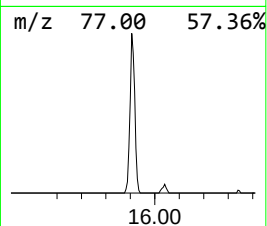
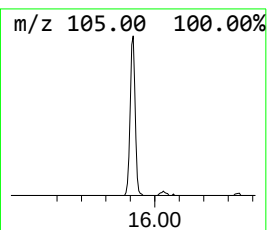
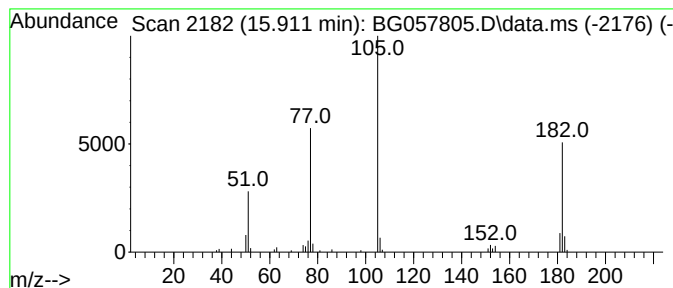
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.911	3.83 ng	81919	Acenaphthene-d10	14.554

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Vinyl benzoate	148	C9H8O2	000769-78-8	47
3			1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47
4			S-Benzoyl(thiohydroxylamine)	153	C7H7NO5	025740-80-1	47
5			Methyl benzilate	242	C15H14O3	000076-89-1	47



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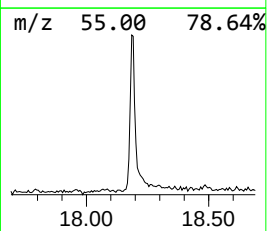
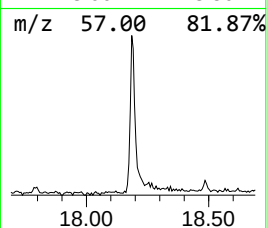
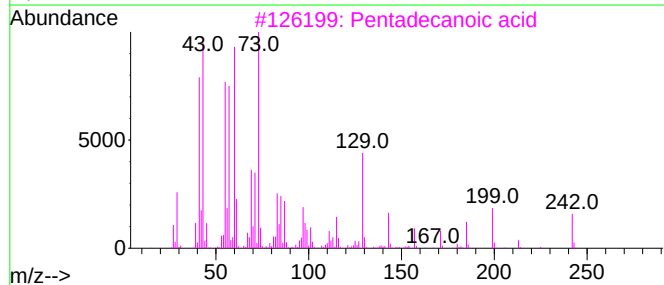
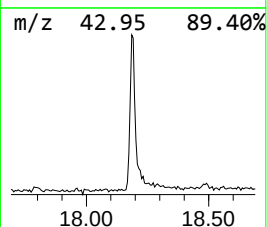
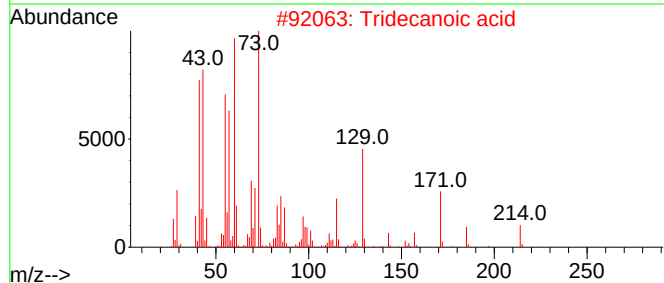
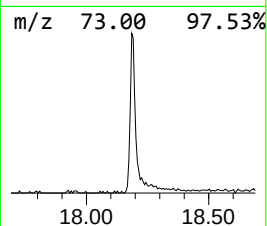
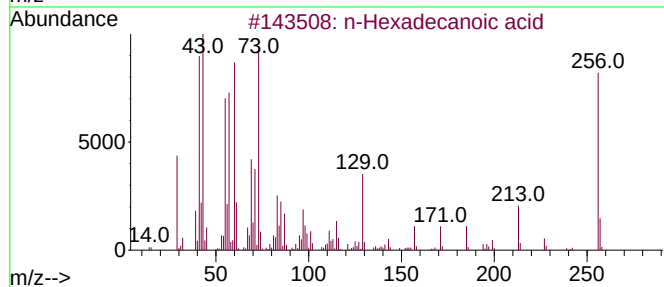
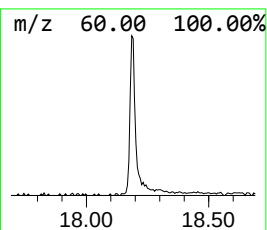
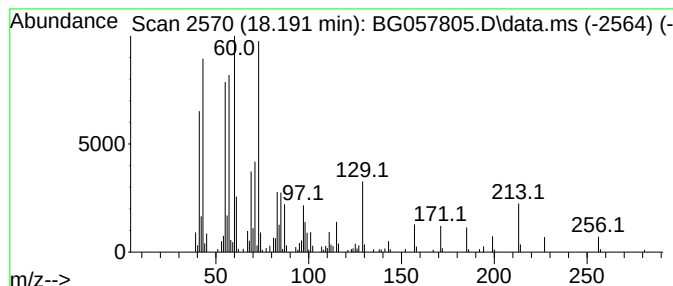
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.191	9.40 ng	281616	Phenanthrene-d10	17.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	90
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	83
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	80



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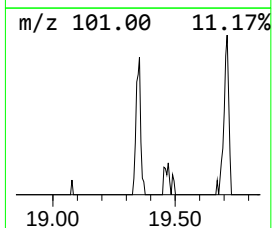
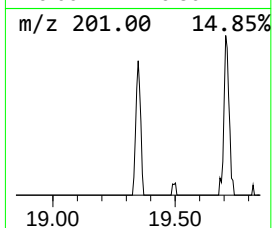
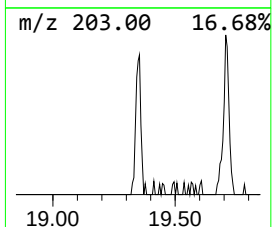
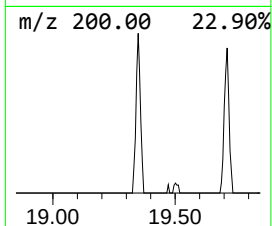
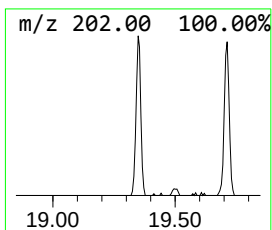
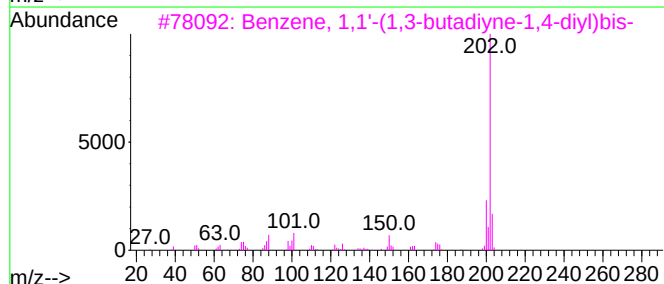
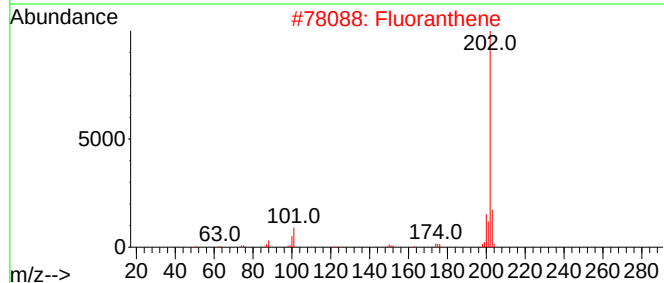
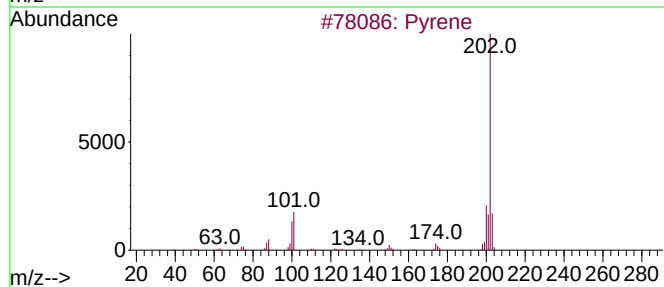
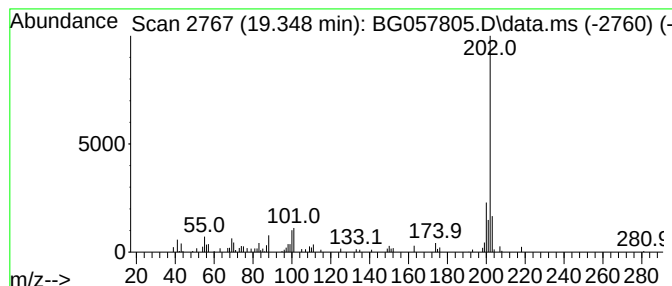
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Peak Number 4 Benzene, 1,1'-(1,3-butadiyn... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.348	2.59 ng	77540	Phenanthrene-d10	17.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pyrene	202	C16H10	000129-00-0	81
2			Fluoranthene	202	C16H10	000206-44-0	81
3			Benzene, 1,1'-(1,3-butadiyne-1,4...	202	C16H10	000886-66-8	76
4			1,4-Pentadiyn-3-one, 1,5-diphenyl-	230	C17H10O	015814-30-9	72
5			2,3-Dichlorobenzo[b]thiophene	202	C8H4Cl2S	1000298-87-9	47



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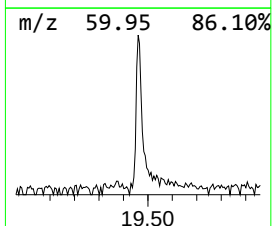
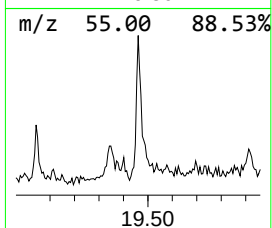
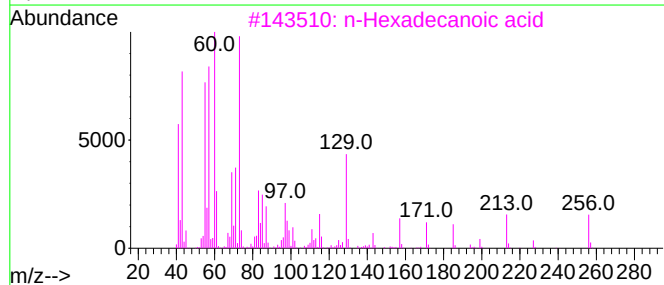
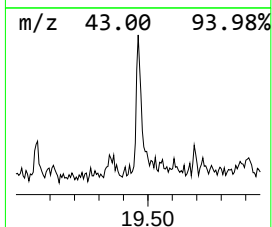
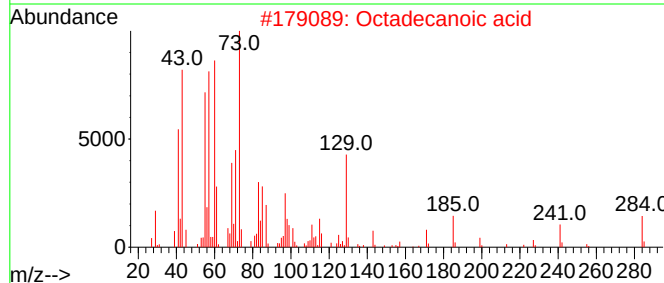
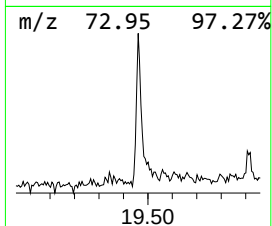
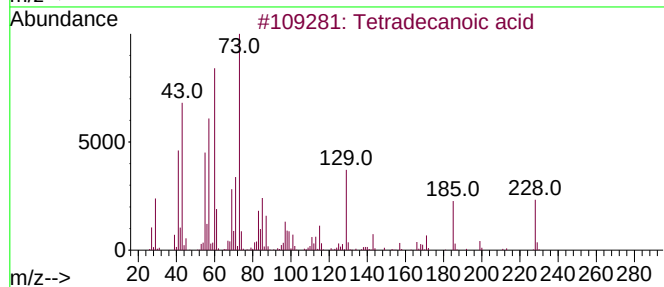
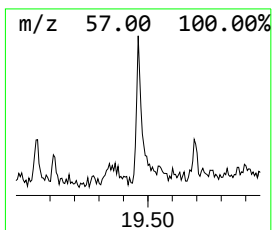
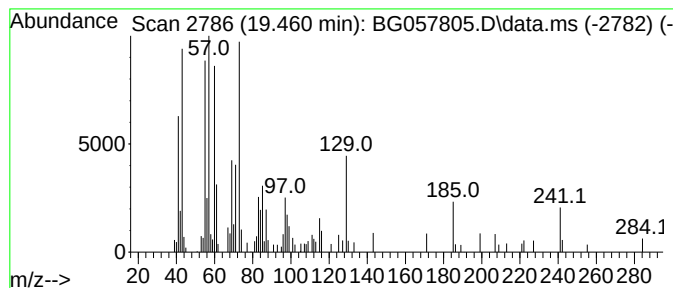
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Tetradecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.460	3.04 ng	104507	Chrysene-d12	21.546

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
2			Octadecanoic acid	284	C18H36O2	000057-11-4	83
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	80
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	58
5			n-Decanoic acid	172	C10H20O2	000334-48-5	58



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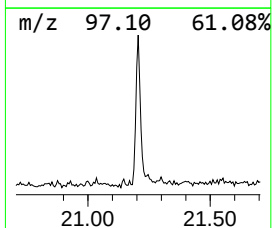
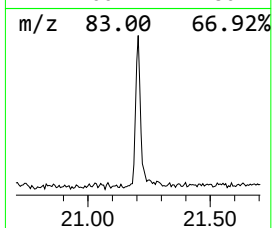
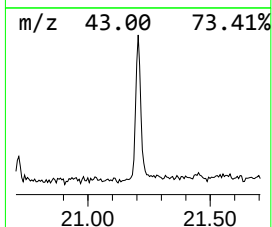
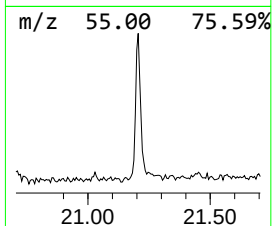
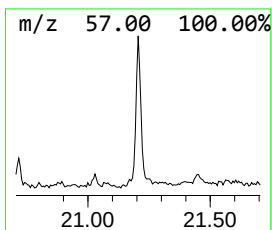
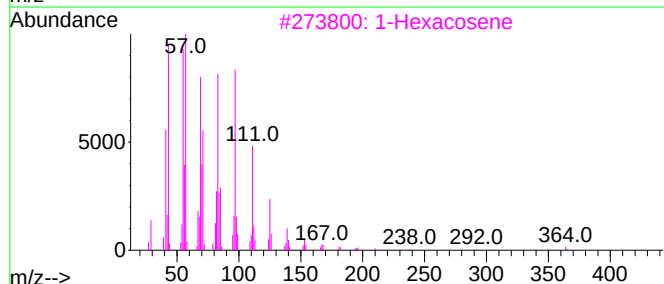
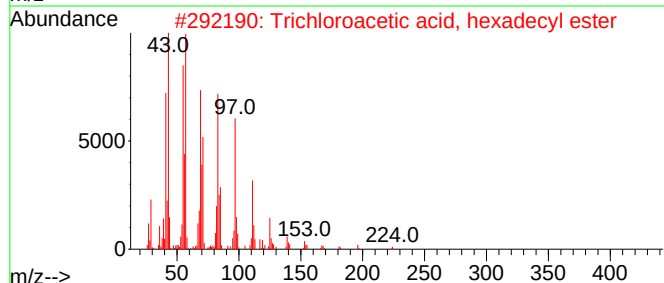
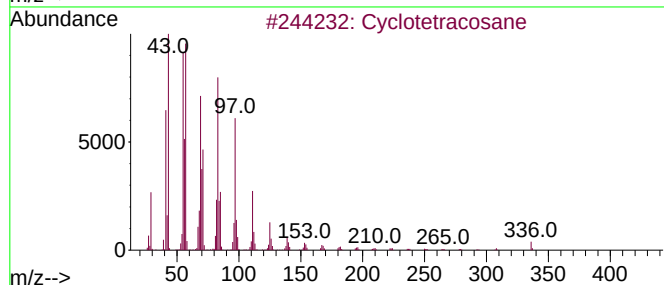
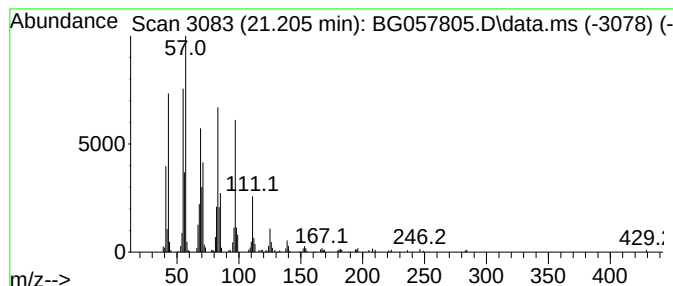
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Cyclotetracosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.205	6.46 ng	221648	Chrysene-d12	21.546

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclotetracosane	336	C24H48	000297-03-0	95
2			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
3			1-Hexacosene	364	C26H52	018835-33-1	94
4			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
5			Cyclooctacosane	392	C28H56	000297-24-5	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062223\
Data File : BG057805.D
Acq On : 22 Jun 2023 11:39
Operator : CG/JU
Sample : 03290-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-2

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

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.024	41.0	ng	356532	1	7.921	173927	20.0
Benzophenone	15.911	3.8	ng	81919	3	14.554	427780	20.0
n-Hexadecanoic ...	18.191	9.4	ng	281616	4	17.298	599203	20.0
Benzene, 1,1'-(...	19.348	2.6	ng	77540	4	17.298	599203	20.0
Tetradecanoic acid	19.460	3.0	ng	104507	5	21.546	686430	20.0
Cyclotetracosane	21.205	6.5	ng	221648	5	21.546	686430	20.0