

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051923\
 Data File : BG057480.D
 Acq On : 19 May 2023 23:41
 Operator : CG/JU
 Sample : 02849-01
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 TP7

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-BG042723.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG057480.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.389	310	315	321	rBV	16191	24516	3.68%	0.591%
2	5.870	391	397	409	rBB	130835	221112	33.19%	5.331%
3	7.010	586	591	597	rBB2	7671	11651	1.75%	0.281%
4	7.498	667	674	684	rBV	143826	255265	38.32%	6.155%
5	8.355	814	820	827	rBB	61354	99475	14.93%	2.398%
6	9.530	1012	1020	1031	rBB	89302	160249	24.06%	3.864%
7	11.193	1295	1303	1312	rBV	76901	139149	20.89%	3.355%
8	13.589	1705	1711	1721	rBV	278170	414730	62.26%	9.999%
9	14.283	1824	1829	1834	rBV	39745	55132	8.28%	1.329%
10	14.911	1930	1936	1940	rBV2	15600	20732	3.11%	0.500%
11	14.970	1940	1946	1951	rBV	136705	219834	33.00%	5.300%
12	15.193	1976	1984	1990	rVB2	16356	20059	3.01%	0.484%
13	15.269	1990	1997	2001	rBV3	7180	11371	1.71%	0.274%
14	16.303	2164	2173	2181	rBV	17187	26844	4.03%	0.647%
15	16.409	2184	2191	2193	rBV3	6463	9546	1.43%	0.230%
16	16.450	2193	2198	2205	rVB	213077	312459	46.91%	7.534%
17	17.707	2405	2412	2419	rBV	200631	297609	44.68%	7.176%
18	18.547	2550	2555	2561	rBV2	9436	16522	2.48%	0.398%
19	18.841	2601	2605	2610	rVB2	25406	31327	4.70%	0.755%
20	20.274	2843	2849	2856	rBV	511162	666109	100.00%	16.060%
21	20.421	2871	2874	2879	rVB4	6283	7981	1.20%	0.192%
22	20.533	2887	2893	2895	rBV5	4916	9897	1.49%	0.239%
23	20.856	2942	2948	2951	rBV6	5199	8765	1.32%	0.211%
24	21.044	2976	2980	2985	rBV6	10768	17207	2.58%	0.415%
25	21.232	3006	3012	3015	rBV7	7613	11484	1.72%	0.277%
26	21.408	3037	3042	3048	rVB	129796	176055	26.43%	4.245%
27	21.573	3065	3070	3076	rBV4	17756	36094	5.42%	0.870%
28	22.013	3138	3145	3155	rVB	193871	327878	49.22%	7.905%
29	22.148	3164	3168	3172	rVB4	6896	9937	1.49%	0.240%
30	22.789	3273	3277	3282	rBV5	8838	12324	1.85%	0.297%
31	23.535	3398	3404	3413	rVB7	9172	18206	2.73%	0.439%
32	24.398	3543	3551	3560	rBV2	29912	64455	9.68%	1.554%
33	25.420	3720	3725	3730	rBV6	9770	20435	3.07%	0.493%
34	25.509	3730	3740	3751	rVB2	103234	316200	47.47%	7.624%
35	26.642	3923	3933	3945	rVB3	27870	86723	13.02%	2.091%
36	26.789	3952	3958	3959	rBV6	6462	10238	1.54%	0.247%

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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-BG042723.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

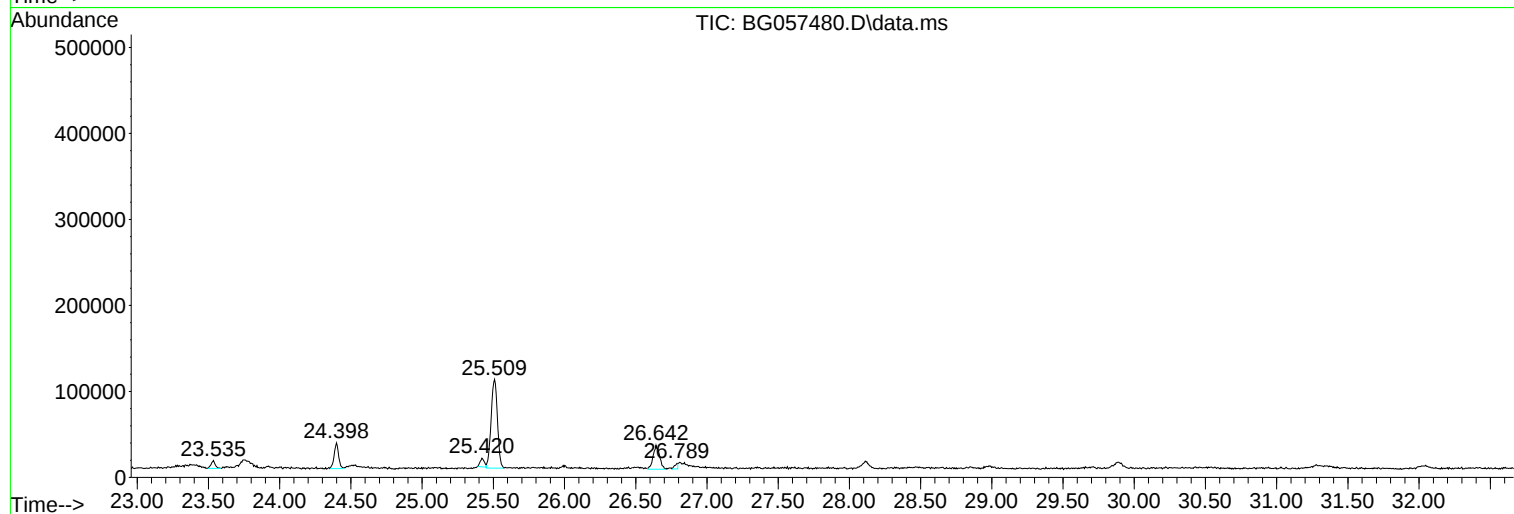
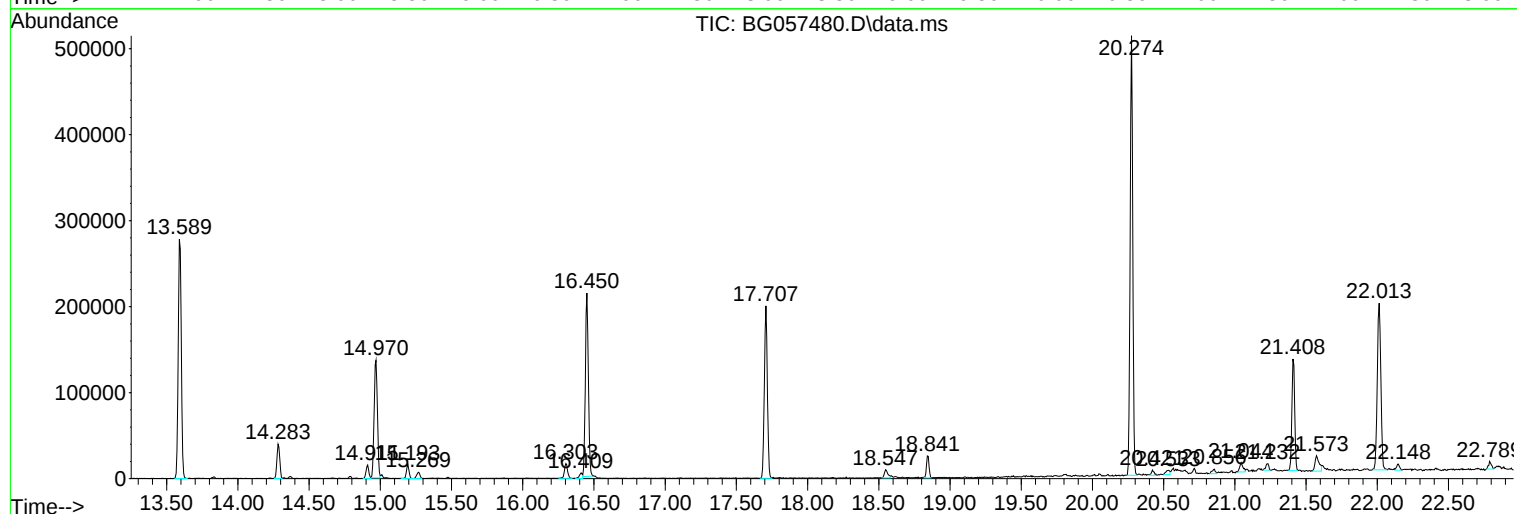
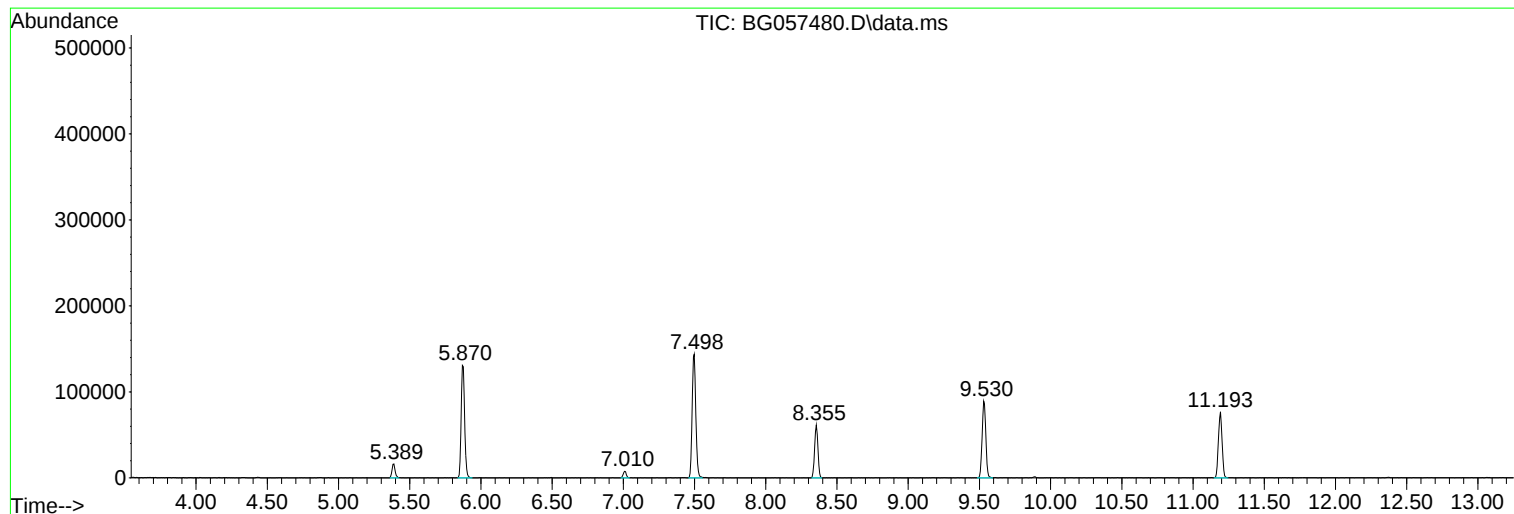
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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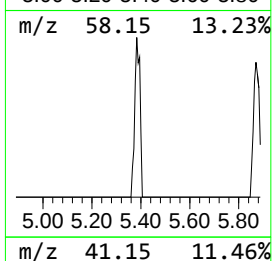
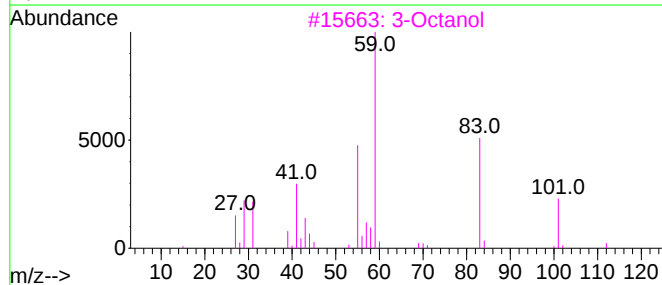
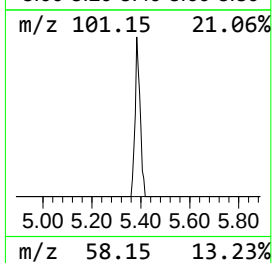
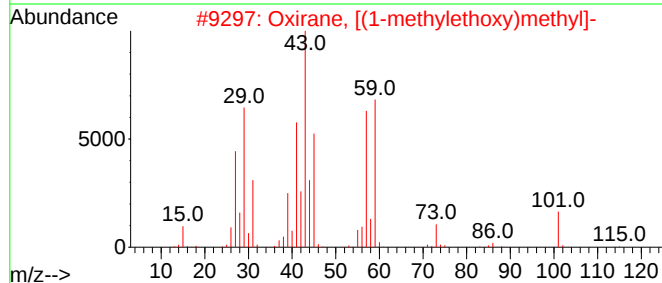
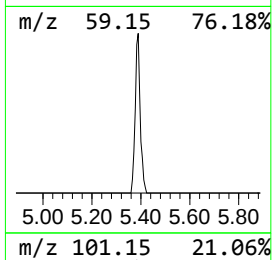
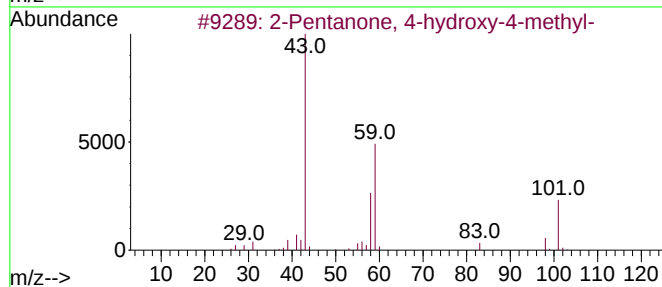
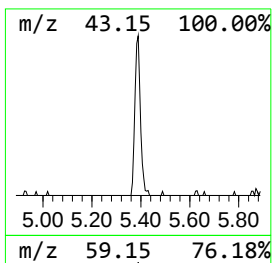
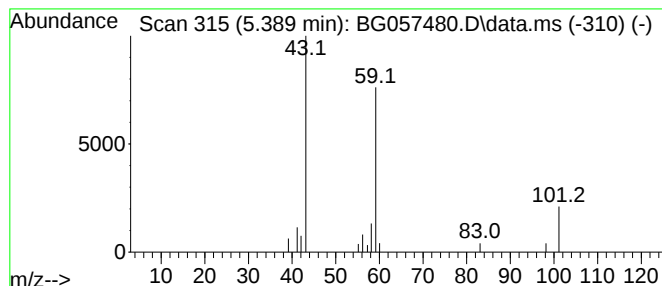
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.389	4.93 ng	24516	1,4-Dichlorobenzene-d4	8.355

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64	
2	Oxirane, [(1-methylethoxy)methyl]-	116	C6H12O2	004016-14-2	43	
3	3-Octanol	130	C8H18O	000589-98-0	39	
4	Silane, trimethyl-	74	C3H10Si	000993-07-7	28	
5	Guanidine	59	CH5N3	000113-00-8	9	



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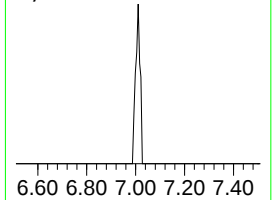
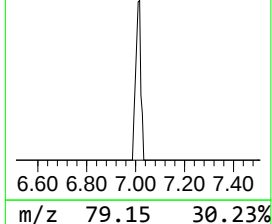
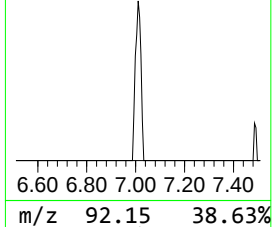
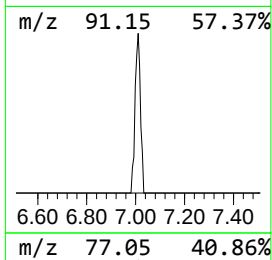
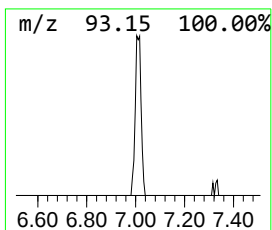
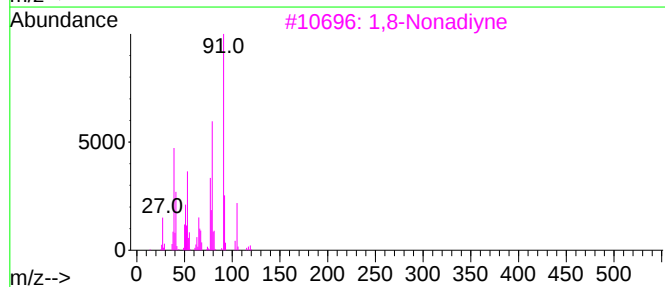
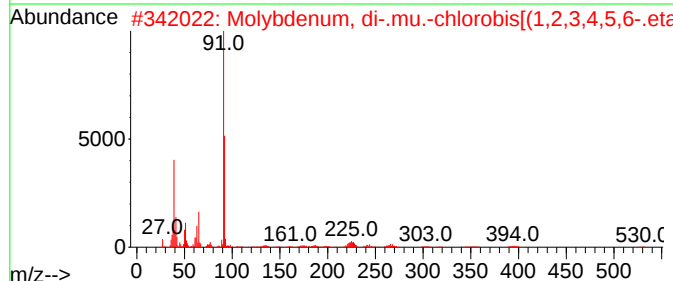
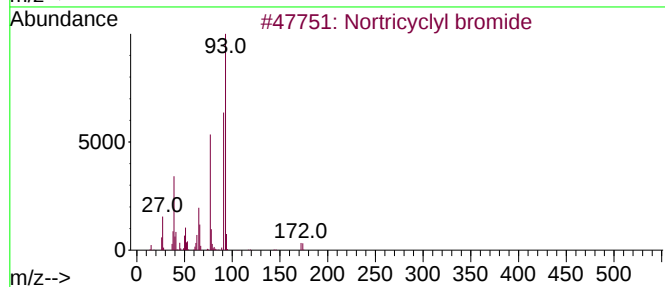
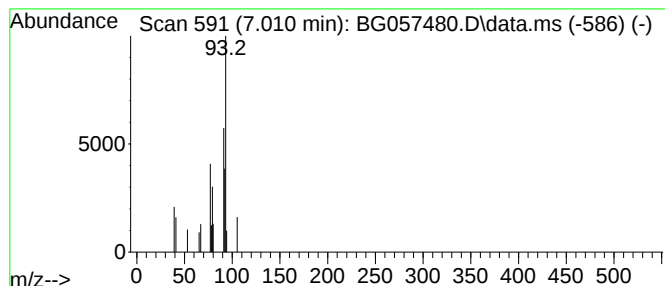
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 unknown7.010 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.010	2.34 ng	11651	1,4-Dichlorobenzene-d4	8.355

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nortricyclyl bromide	172	C7H9Br	1000342-32-2	33
2			Molybdenum, di-.mu.-chlorobis[(1...	532	C20H26Cl2Mo2	035625-66-2	9
3			1,8-Nonadiyne	120	C9H12	002396-65-8	9
4			Toluene	92	C7H8	000108-88-3	7
5			1,5-Heptadien-3-yne	92	C7H8	003511-27-1	7



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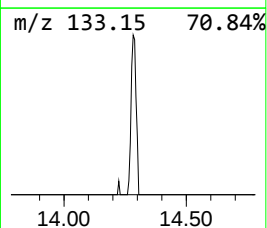
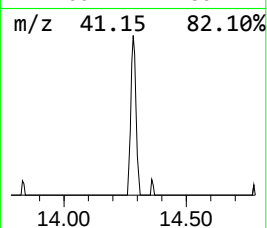
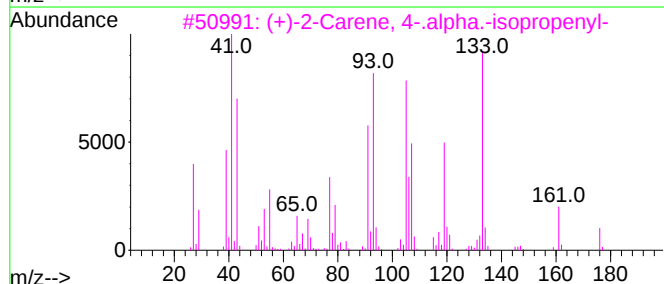
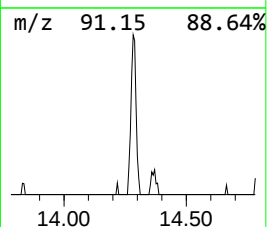
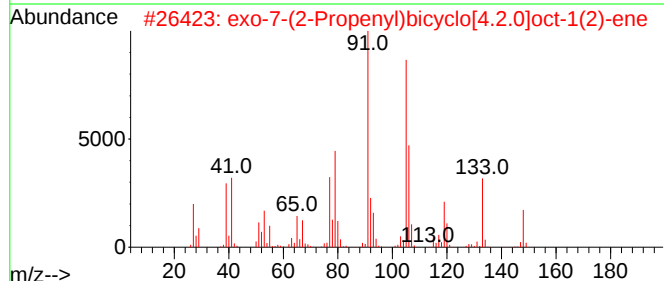
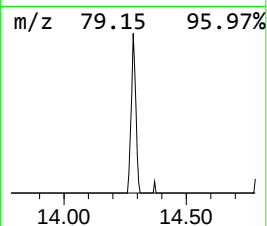
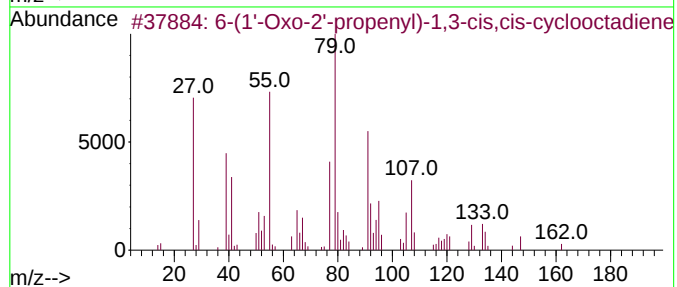
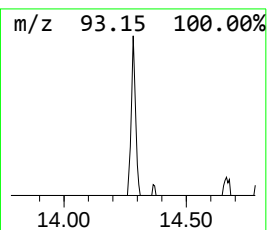
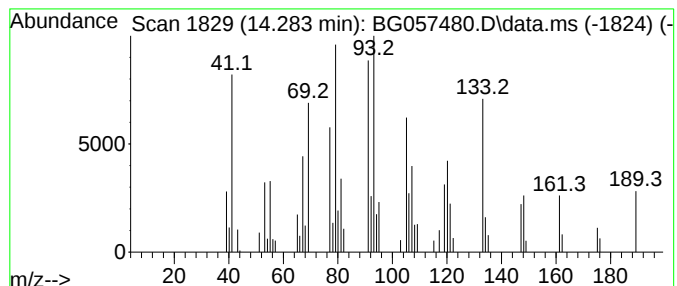
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 unknown14.283 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.283	5.02 ng	55132	Acenaphthene-d10	14.970

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	6-(1'-Oxo-2'-propenyl)-1,3-cis,c...	162	C11H14O	138146-05-1	42		
2	exo-7-(2-Propenyl)bicyclo[4.2.0]...	148	C11H16	1000200-97-5	38		
3	(+)-2-Carene, 4-.alpha.-isopropen...	176	C13H20	1000151-26-0	38		
4	Bicyclo[4.2.1]nona-2,4-dien-9-en...	162	C11H14O	138146-02-8	35		
5	Bicyclo[5.1.0]octane, 8-methylene-	122	C9H14	054211-15-3	30		



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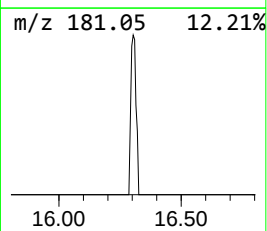
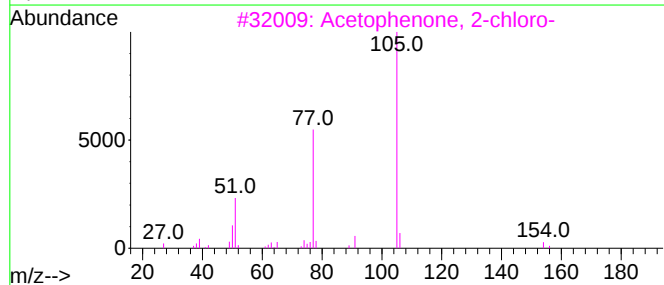
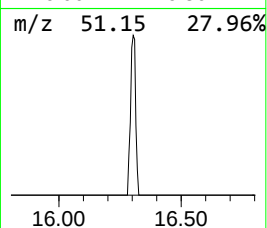
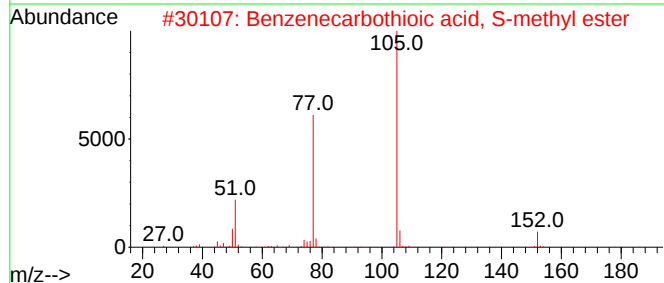
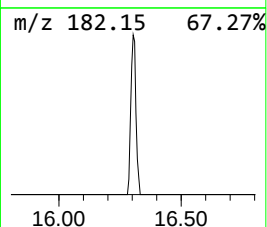
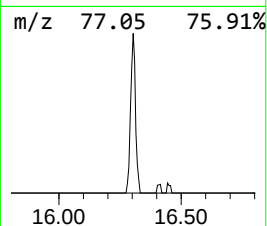
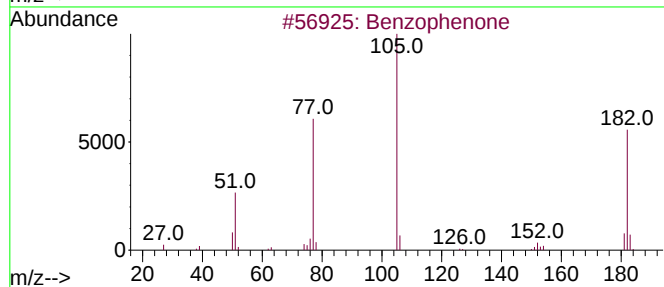
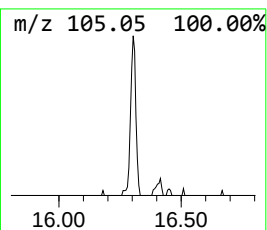
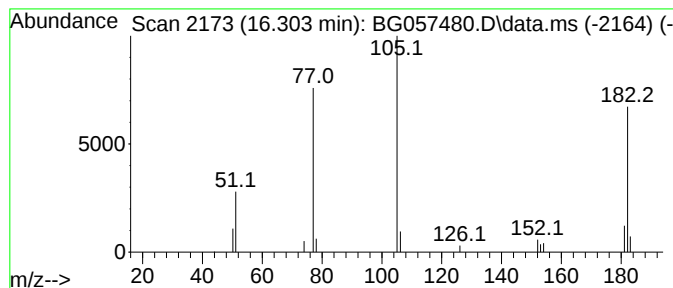
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Peak Number 4 Benzophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.303	2.44 ng	26844	Acenaphthene-d10	14.970

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	91
2			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	52
3			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	52
4			Ethanone, 2,2,2-trifluoro-1-phenyl-	174	C8H5F3O	000434-45-7	50
5			Benzoyl isothiocyanate	163	C8H5NOS	000532-55-8	50



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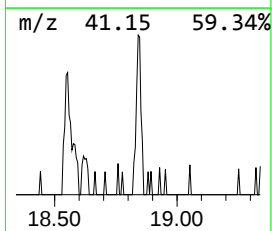
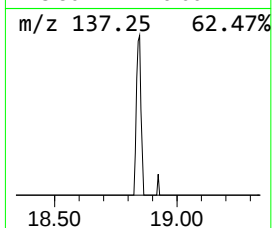
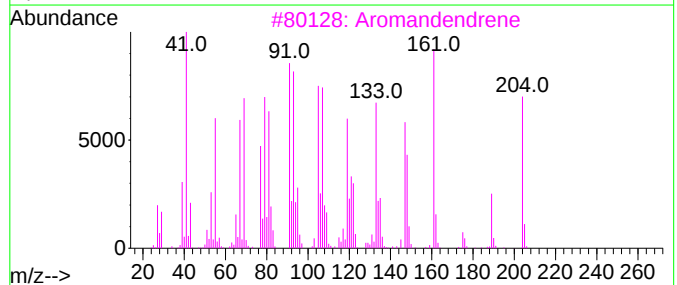
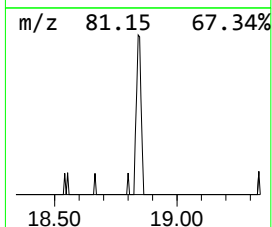
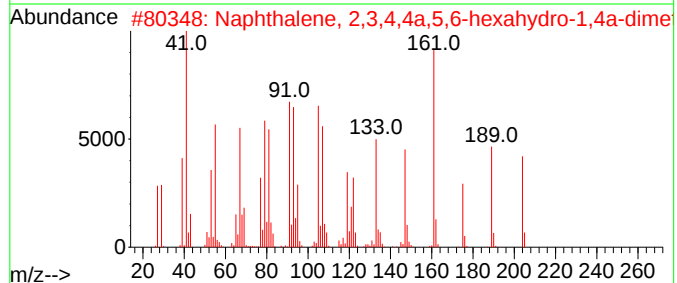
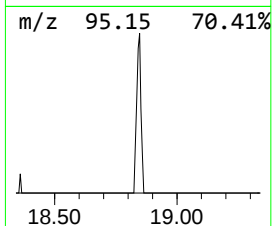
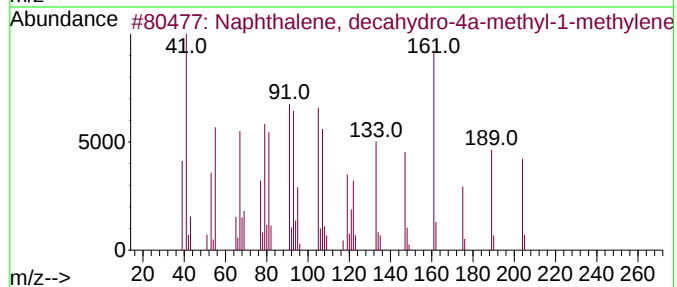
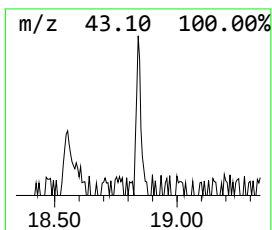
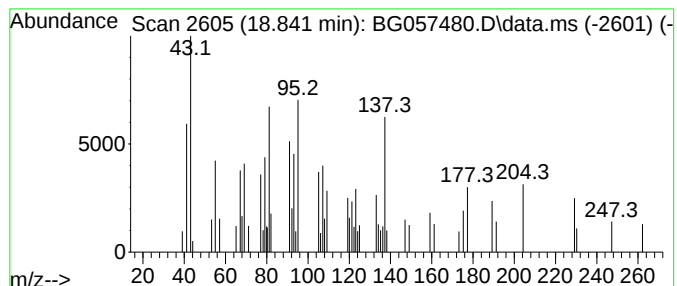
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Peak Number 5 Naphthalene, decahydro-4a-m... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.841	2.11 ng	31327	Phenanthrene-d10	17.707

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, decahydro-4a-methyl...	204	C15H24	017066-67-0	52
2			Naphthalene, 2,3,4,4a,5,6-hexahy...	204	C15H24	000473-14-3	52
3			Aromandendrene	204	C15H24	000489-39-4	49
4			Alloaromadendrene	204	C15H24	025246-27-9	48
5			Petasitene	204	C15H24	443124-67-2	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051923\
Data File : BG057480.D
Acq On : 19 May 2023 23:41
Operator : CG/JU
Sample : 02849-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP7

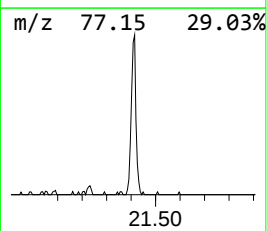
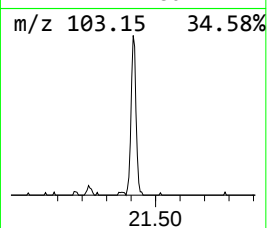
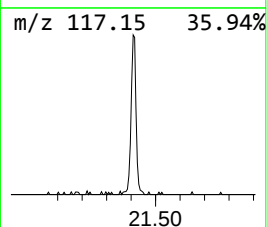
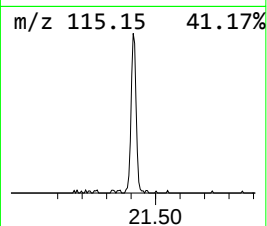
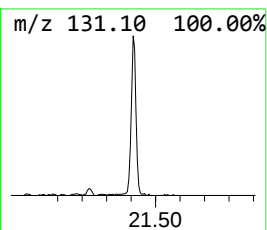
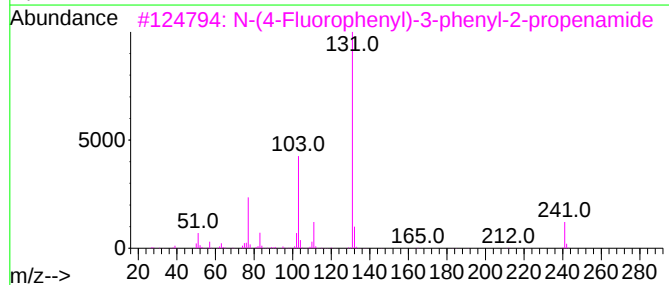
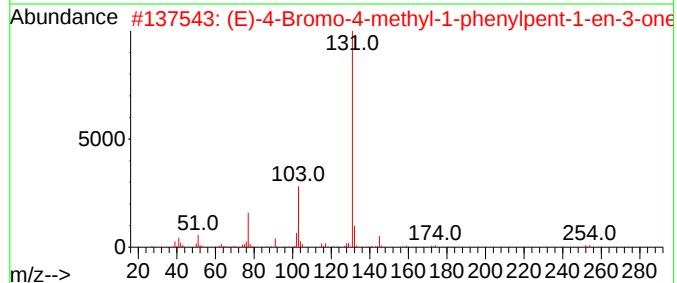
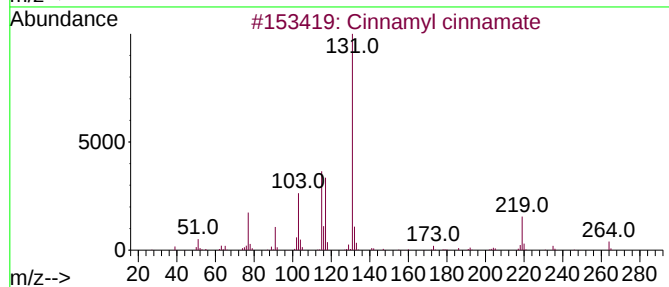
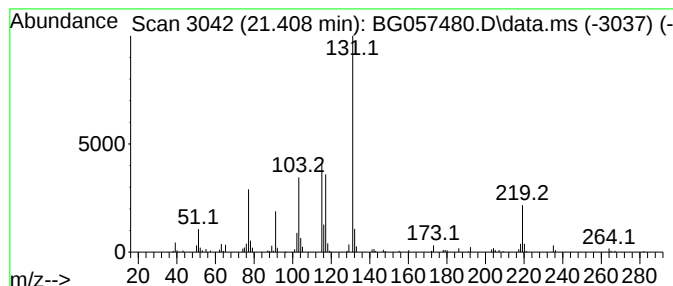
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Cinnamyl cinnamate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.408	10.74 ng	176055	Chrysene-d12	22.013

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cinnamyl cinnamate	264	C18H16O2	000122-69-0	91
2			(E)-4-Bromo-4-methyl-1-phenylpen...	252	C12H13BrO	1000443-02-8	47
3			N-(4-Fluorophenyl)-3-phenyl-2-pr...	241	C15H12FNO	019358-27-1	43
4			2-Propenoic acid, 3-phenyl-, phe...	224	C15H12O2	025695-77-6	43
5			2,2-Dimethyl-1-(2-vinylphenyl)pr...	188	C13H16O	1000210-99-9	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051923\
Data File : BG057480.D
Acq On : 19 May 2023 23:41
Operator : CG/JU
Sample : 02849-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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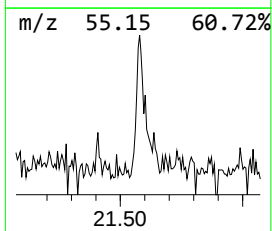
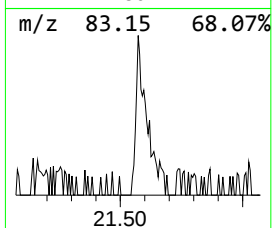
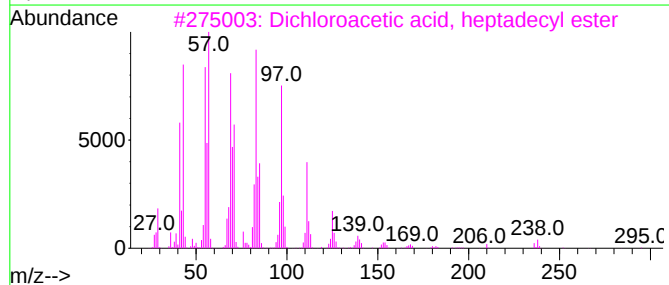
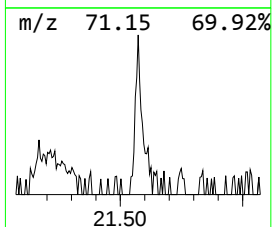
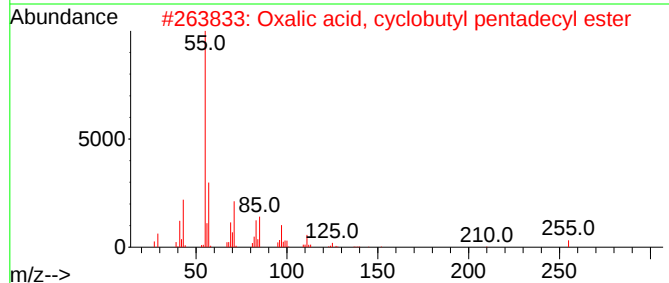
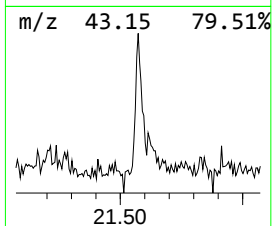
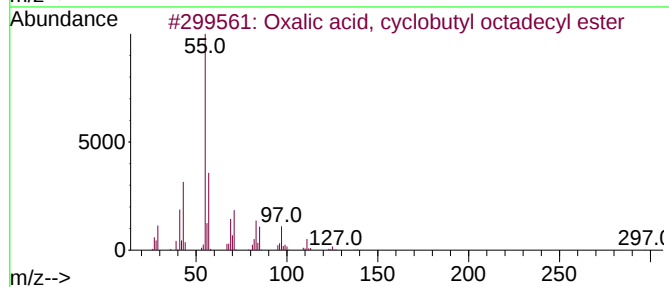
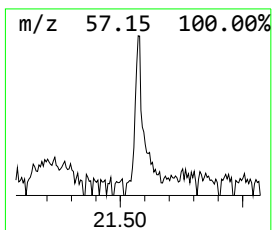
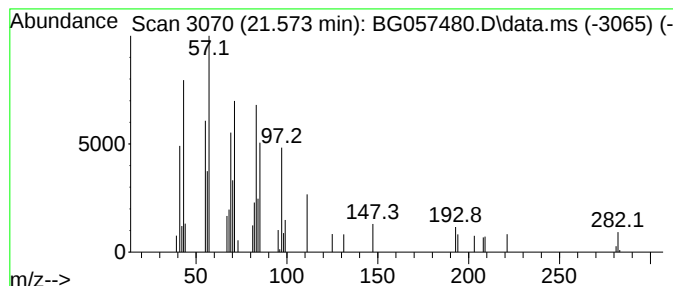
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Oxalic acid, cyclobutyl oct... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.573	2.20 ng	36094	Chrysene-d12	22.013

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxalic acid, cyclobutyl octadecyl...	396	C24H44O4	1000309-70-8	72
2			Oxalic acid, cyclobutyl pentadecyl...	354	C21H38O4	1010309-70-5	72
3			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	64
4			Tetrapentacontane, 1,54-dibromo-	915	C54H108Br2	1000156-09-4	64
5			Acetic acid, chloro-, octadecyl ...	346	C20H39ClO2	005348-82-3	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051923\
Data File : BG057480.D
Acq On : 19 May 2023 23:41
Operator : CG/JU
Sample : 02849-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP7

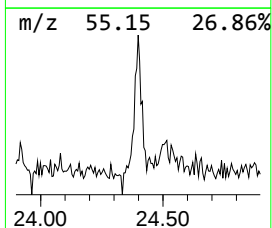
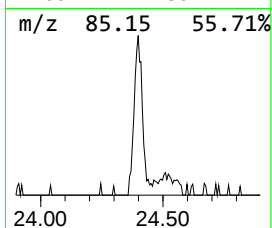
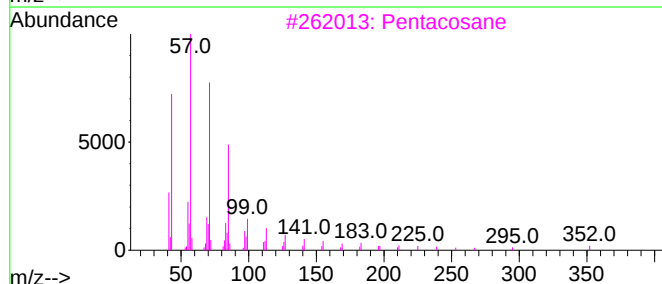
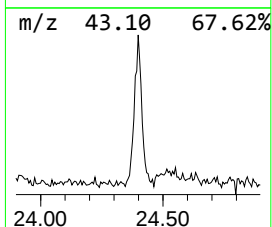
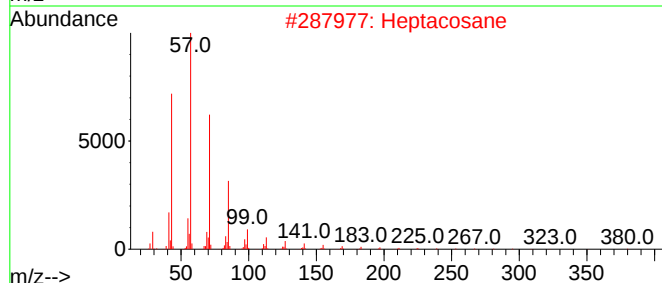
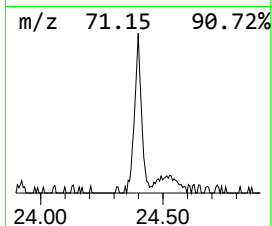
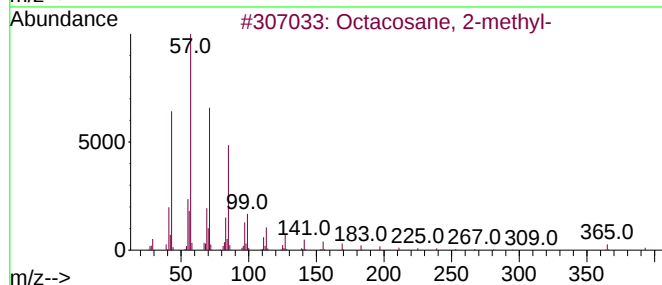
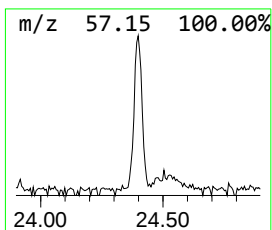
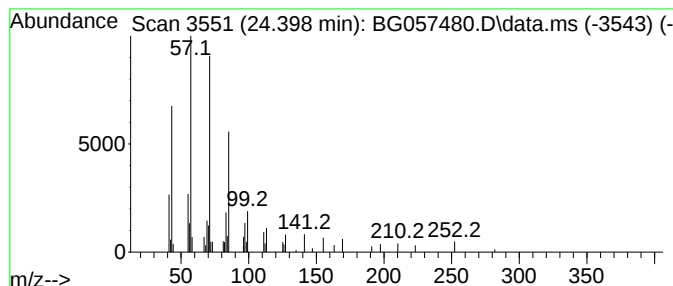
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octacosane, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.398	4.08 ng	64455	Perylene-d12	25.509

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octacosane, 2-methyl-	408	C29H60	001560-98-1	87
2		Heptacosane	380	C27H56	000593-49-7	87
3		Pentacosane	352	C25H52	000629-99-2	87
4		Heneicosane	296	C21H44	000629-94-7	87
5		triacontane	422	C30H62	000638-68-6	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051923\
Data File : BG057480.D
Acq On : 19 May 2023 23:41
Operator : CG/JU
Sample : 02849-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP7

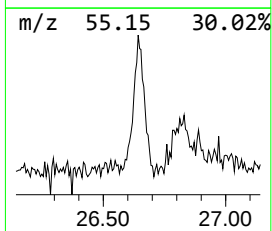
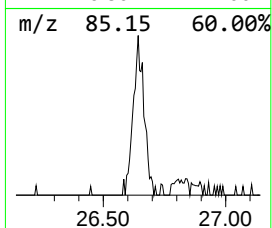
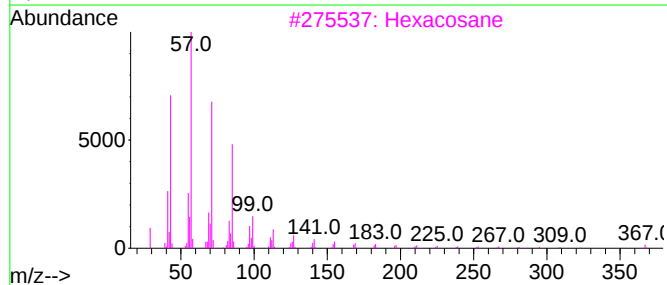
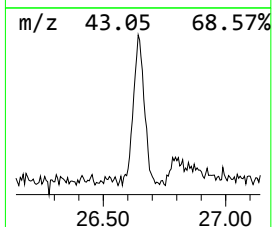
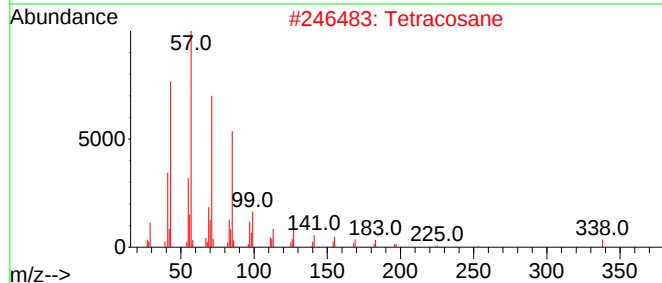
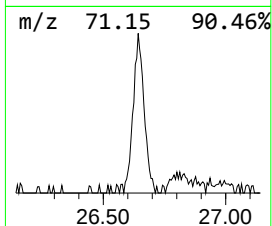
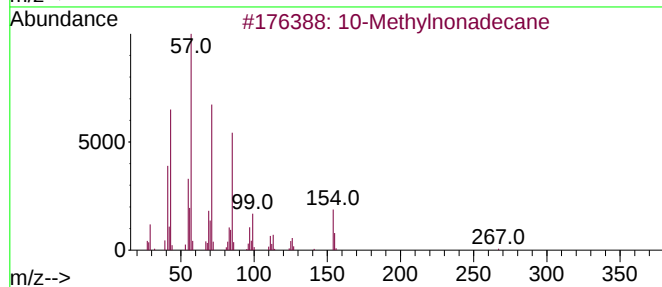
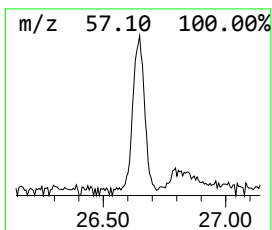
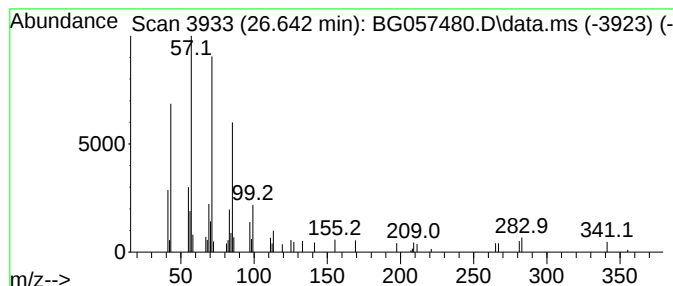
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 10-Methylnonadecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.642	5.49 ng	86723	Perylene-d12	25.509

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		10-Methylnonadecane	282	C20H42	056862-62-5	83
2		Tetracosane	338	C24H50	000646-31-1	83
3		Hexacosane	366	C26H54	000630-01-3	83
4		4-Methylheneicosane	310	C22H46	025117-29-7	83
5		Octacosane	394	C28H58	000630-02-4	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051923\
Data File : BG057480.D
Acq On : 19 May 2023 23:41
Operator : CG/JU
Sample : 02849-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP7

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042723.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
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unknown7.010	7.010	2.3	ng	11651	1	8.355	99475	20.0
unknown14.283	14.283	5.0	ng	55132	3	14.970	219834	20.0
Benzophenone	16.303	2.4	ng	26844	3	14.970	219834	20.0
Naphthalene, de...	18.841	2.1	ng	31327	4	17.707	297609	20.0
Cinnamyl cinnamate	21.408	10.7	ng	176055	5	22.013	327878	20.0
Oxalic acid, cy...	21.573	2.2	ng	36094	5	22.013	327878	20.0
Octacosane, 2-m...	24.398	4.1	ng	64455	6	25.509	316200	20.0
10-Methylnonade...	26.642	5.5	ng	86723	6	25.509	316200	20.0