

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041122\
 Data File : BG053105.D
 Acq On : 11 Apr 2022 17:35
 Operator : CG/JU
 Sample : N2317-07
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 NORTH-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-BG040822.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG053105.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.210	303	310	318	rVB	31421	47965	2.66%	0.433%
2	5.686	384	391	402	rBV	434658	718518	39.81%	6.486%
3	6.808	575	582	592	rVB	34072	54380	3.01%	0.491%
4	7.278	654	662	671	rBV	484791	848898	47.03%	7.663%
5	8.118	799	805	813	rVB	106221	185113	10.26%	1.671%
6	9.281	993	1003	1014	rBV	290488	541520	30.00%	4.888%
7	10.932	1276	1284	1293	rBV	148486	270887	15.01%	2.445%
8	13.364	1691	1698	1708	rVB	724310	1165112	64.55%	10.518%
9	13.628	1738	1743	1751	rBV2	18240	27251	1.51%	0.246%
10	14.157	1828	1833	1840	rVB3	14237	19516	1.08%	0.176%
11	14.703	1917	1926	1929	rBV	304684	471894	26.14%	4.260%
12	14.739	1929	1932	1940	rVB	246093	387609	21.47%	3.499%
13	14.991	1969	1975	1982	rBV2	23735	31167	1.73%	0.281%
14	16.225	2176	2185	2194	rVV	727085	1144271	63.39%	10.330%
15	16.577	2240	2245	2254	rBV4	20060	35181	1.95%	0.318%
16	17.482	2393	2399	2410	rVB	354499	546145	30.26%	4.930%
17	18.363	2545	2549	2557	rBV5	31712	52526	2.91%	0.474%
18	20.084	2836	2842	2848	rBV	1392270	1805047	100.00%	16.295%
19	20.243	2864	2869	2873	rVB	38682	48153	2.67%	0.435%
20	20.384	2885	2893	2896	rBV7	23043	37999	2.11%	0.343%
21	21.212	3028	3034	3044	rVB	535804	742639	41.14%	6.704%
22	21.394	3059	3065	3075	rBV	128280	253019	14.02%	2.284%
23	21.764	3121	3128	3137	rBV2	360235	609300	33.76%	5.500%
24	22.604	3262	3271	3281	rBV8	42456	120360	6.67%	1.087%
25	22.834	3306	3310	3319	rBV10	10525	23514	1.30%	0.212%
26	23.474	3416	3419	3425	rVB3	12984	22651	1.25%	0.204%
27	23.638	3444	3447	3454	rVB8	12462	22194	1.23%	0.200%
28	24.108	3522	3527	3533	rVB2	31884	67510	3.74%	0.609%
29	25.066	3678	3690	3703	rVB2	211255	622169	34.47%	5.616%
30	25.618	3778	3784	3792	rVB8	17696	44580	2.47%	0.402%
31	26.247	3884	3891	3901	rVB4	31202	90197	5.00%	0.814%
32	30.552	4616	4624	4625	rBV8	9060	20242	1.12%	0.183%

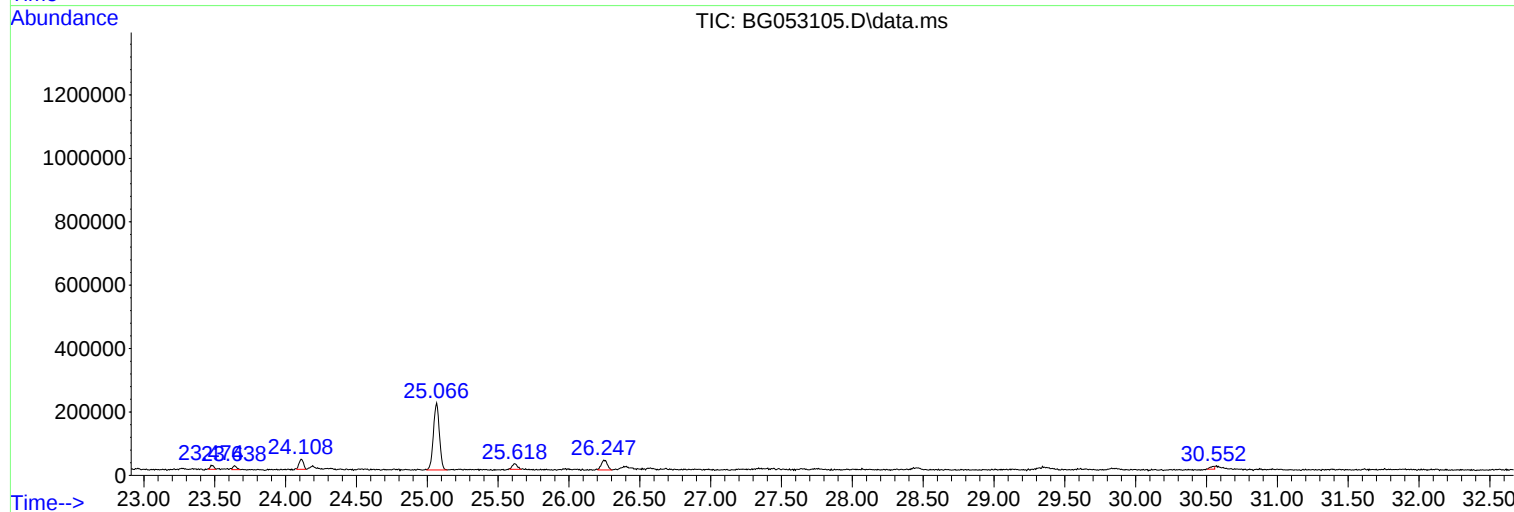
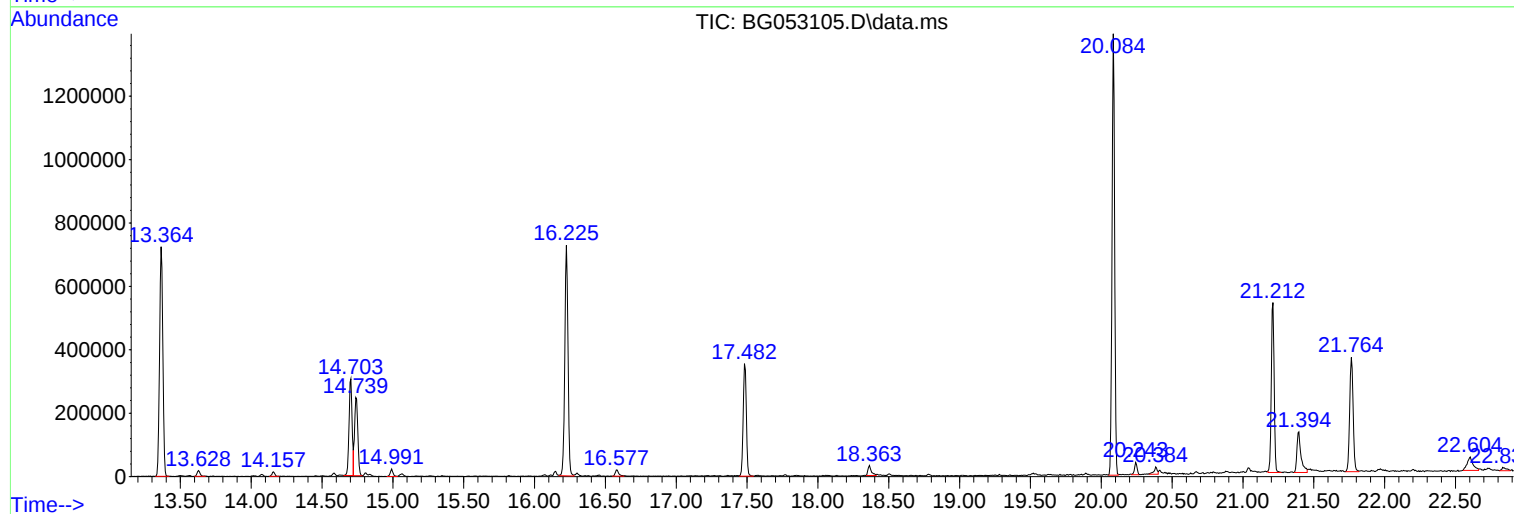
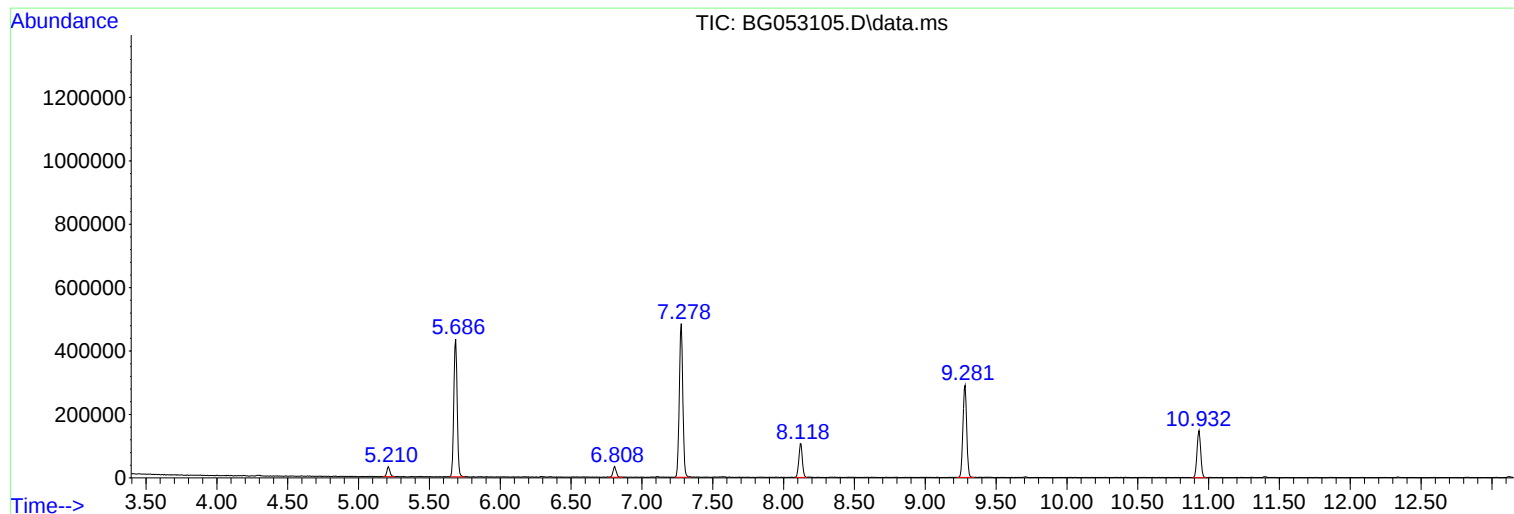
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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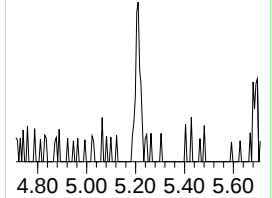
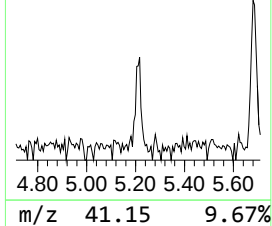
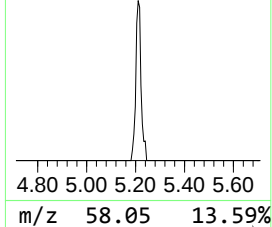
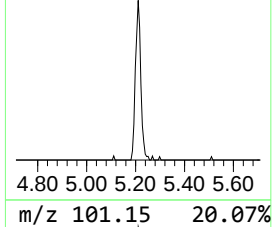
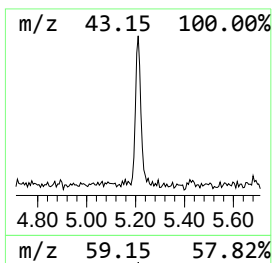
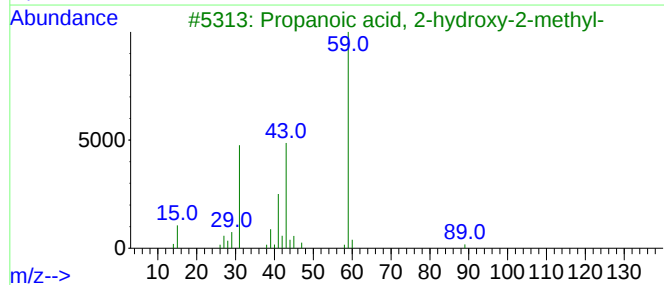
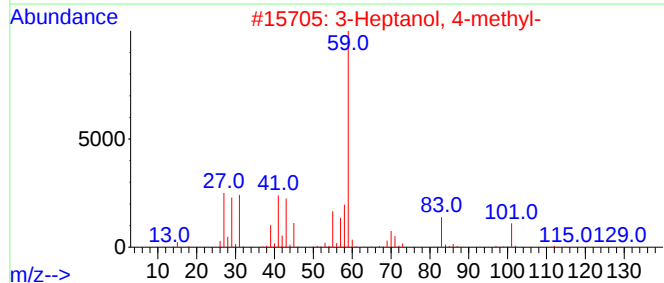
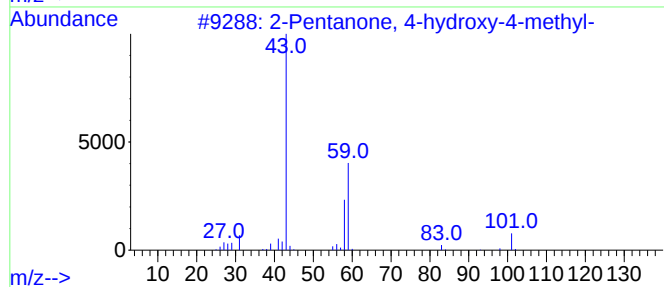
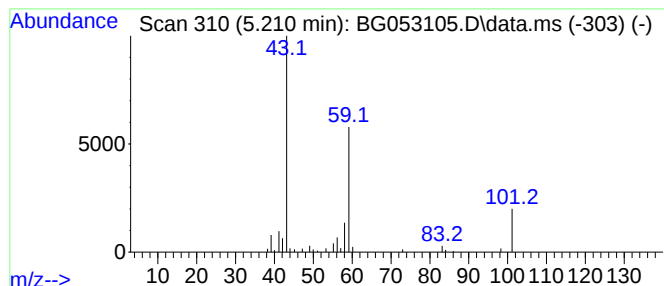
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.210	5.18 ng	47965	1,4-Dichlorobenzene-d4	8.124

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			3-Heptanol, 4-methyl-	130	C8H18O	014979-39-6	28
3			Propanoic acid, 2-hydroxy-2-methyl-	104	C4H8O3	000594-61-6	17
4			Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	12
5			Butane	58	C4H10	000106-97-8	9



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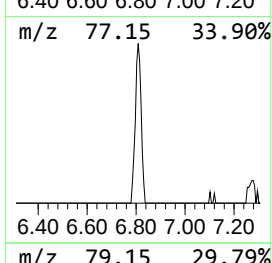
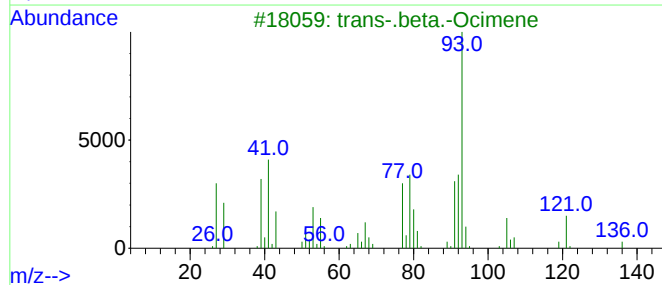
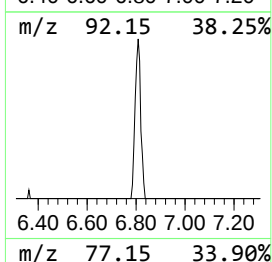
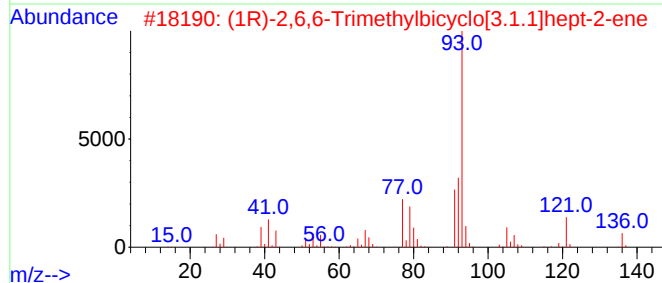
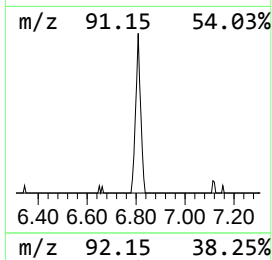
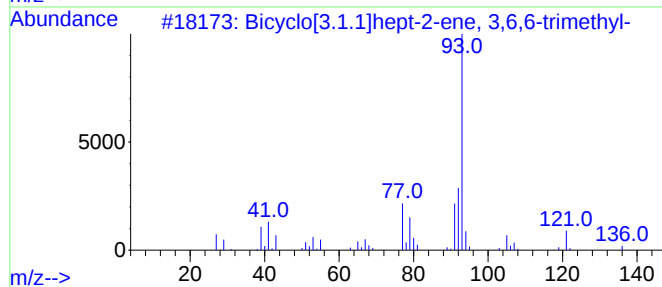
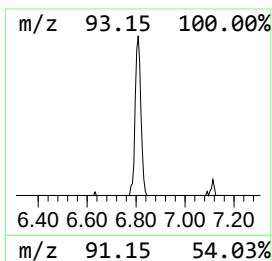
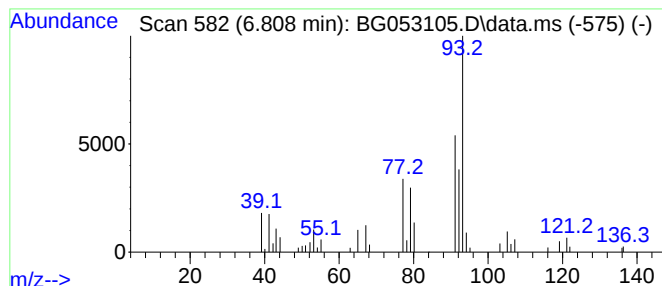
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Bicyclo[3.1.1]hept-2-ene, 3... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.808	5.88 ng	54380	1,4-Dichlorobenzene-d4	8.124

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bicyclo[3.1.1]hept-2-ene, 3,6,6-...	136	C10H16	004889-83-2	91
2			(1R)-2,6,6-Trimethylbicyclo[3.1....	136	C10H16	007785-70-8	91
3			trans-.beta.-Ocimene	136	C10H16	003779-61-1	90
4			(1S)-2,6,6-Trimethylbicyclo[3.1....	136	C10H16	007785-26-4	86
5			Bicyclo[3.1.0]hex-2-ene, 2-methy...	136	C10H16	002867-05-2	86



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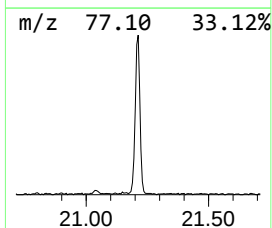
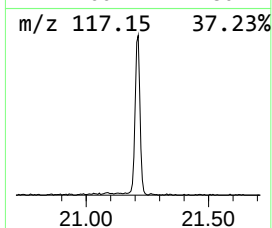
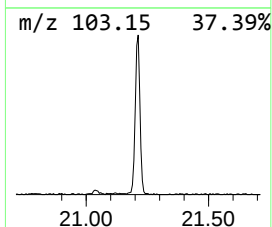
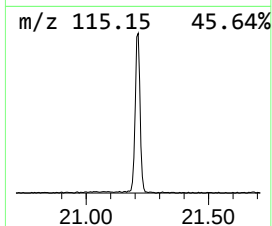
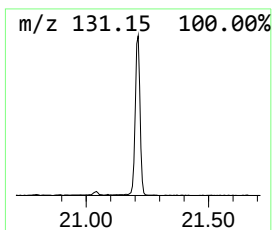
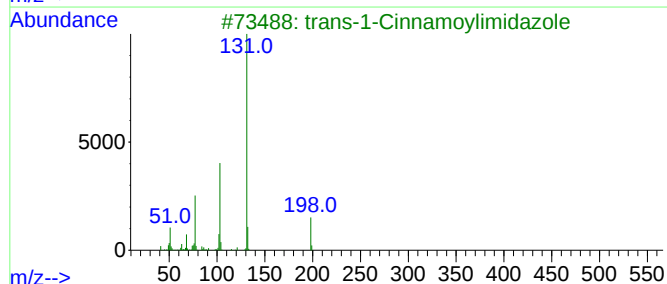
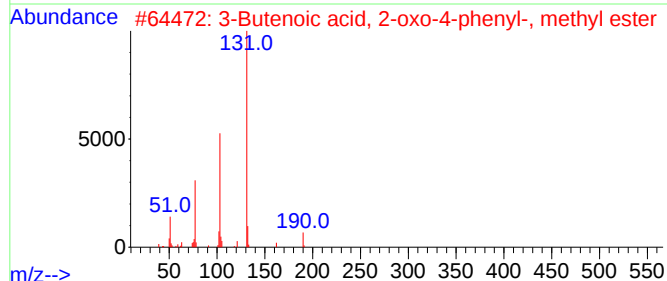
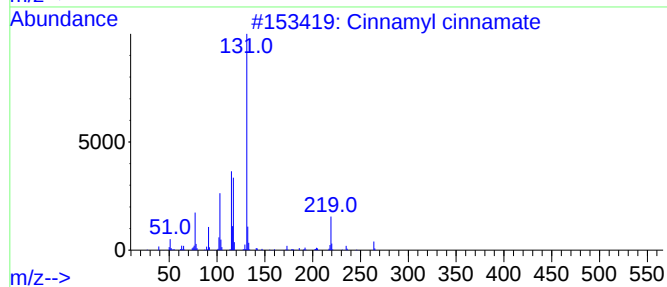
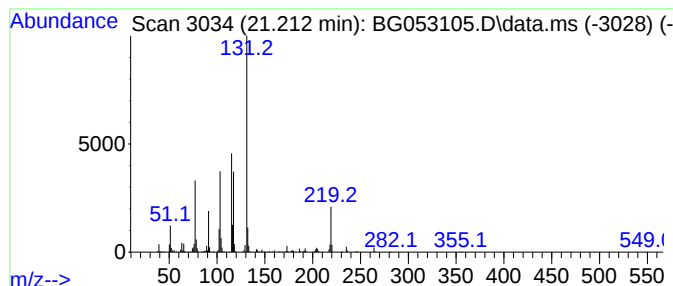
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Cinnamyl cinnamate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.212	24.38 ng	742639	Chrysene-d12	21.764

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cinnamyl cinnamate	264	C18H16O2	000122-69-0	91
2			3-Butenoic acid, 2-oxo-4-phenyl-...	190	C11H10O3	1000142-22-4	49
3			trans-1-Cinnamoylimidazole	198	C12H10N2O	001138-15-4	47
4			N-(p-Vinylbenzoyl)-l-alanine	219	C12H13NO3	139184-60-4	47
5			N-(4-Fluorophenyl)-3-phenyl-2-pr...	241	C15H12FNO	019358-27-1	47



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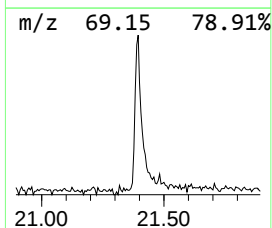
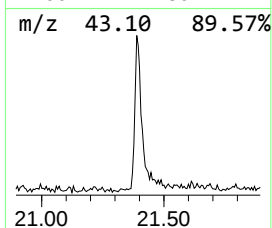
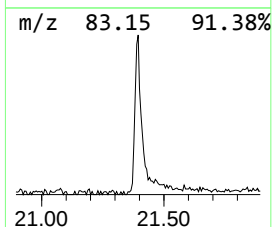
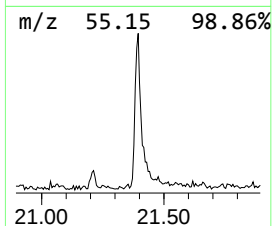
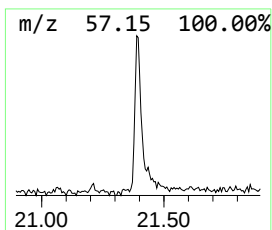
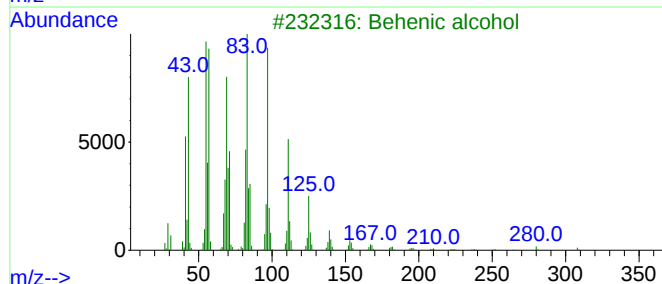
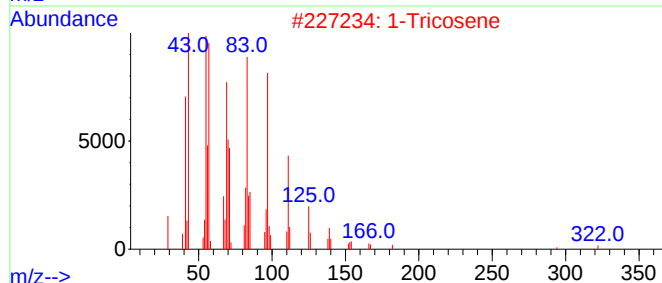
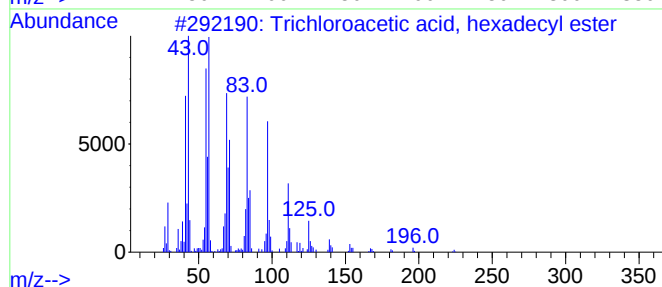
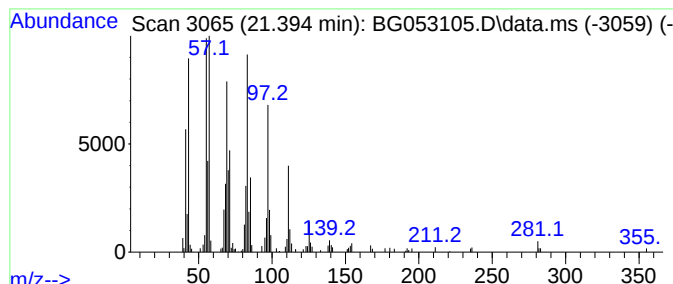
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Trichloroacetic acid, hexad... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.394	8.31 ng	253019	Chrysene-d12	21.764

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
2			1-Tricosene	322	C23H46	018835-32-0	91
3			Behenic alcohol	326	C22H46O	000661-19-8	91
4			1-Heptacosanol	396	C27H56O	002004-39-9	91
5			Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	91



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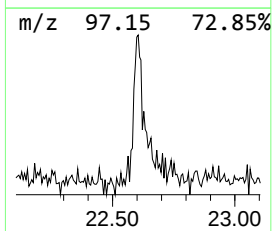
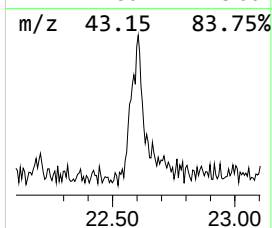
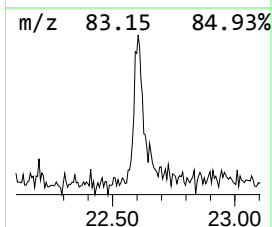
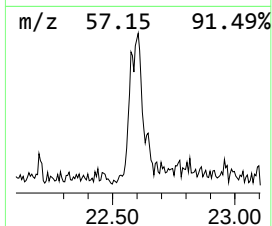
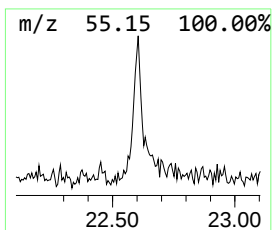
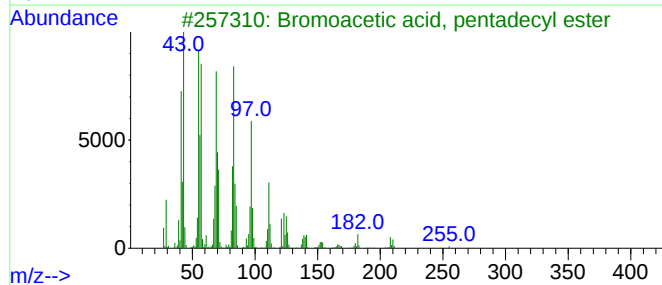
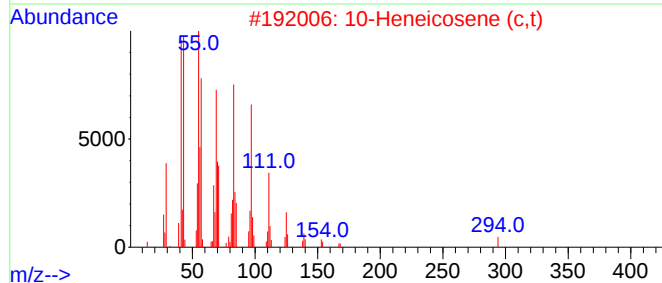
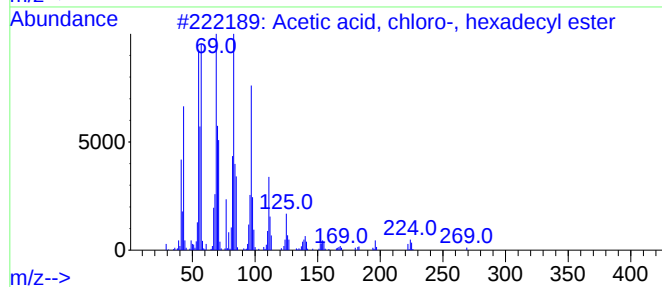
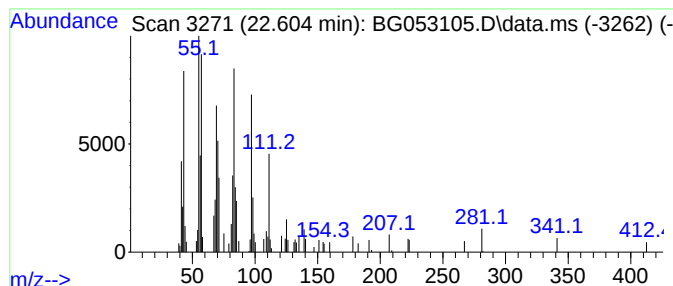
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Peak Number 5 Acetic acid, chloro-, hexad... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.604	3.95 ng	120360	Chrysene-d12	21.764

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, chloro-, hexadecyl ...	318	C18H35ClO2	052132-58-8	87
2			10-Heneicosene (c,t)	294	C21H42	095008-11-0	87
3			Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	87
4			9-Nonadecene	266	C19H38	031035-07-1	87
5			1-Hexadecanol	242	C16H34O	036653-82-4	87



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NORTH-2

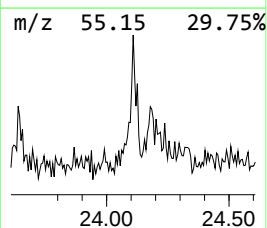
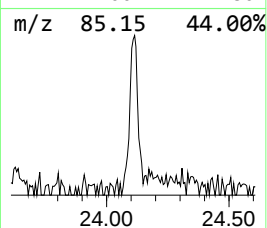
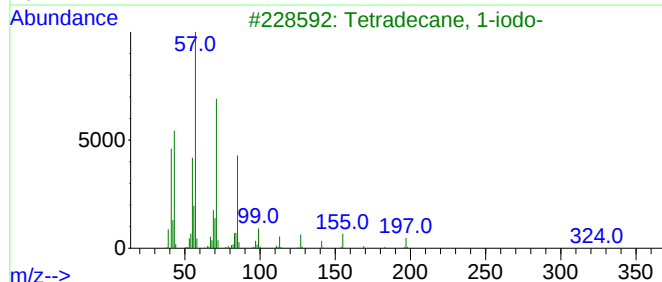
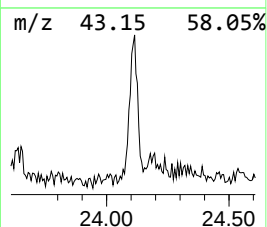
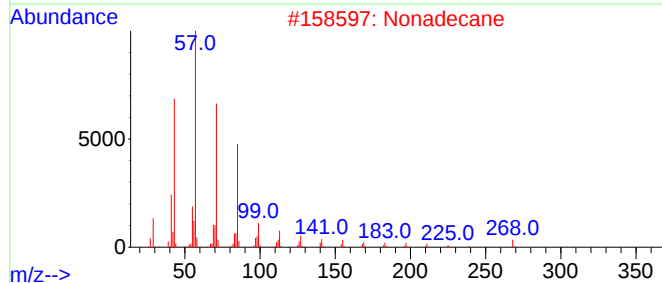
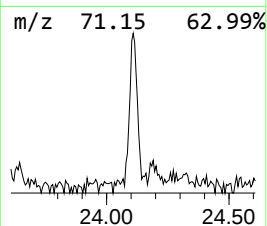
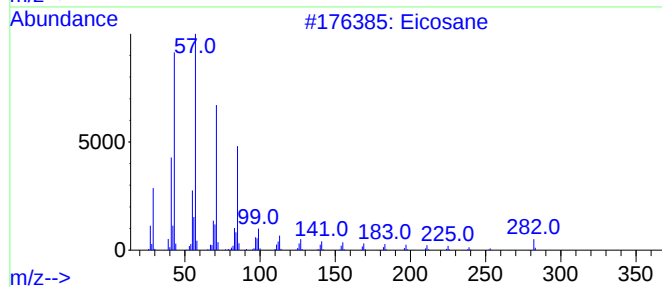
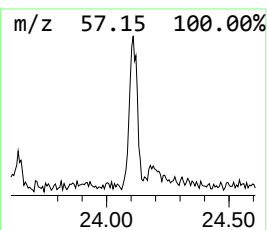
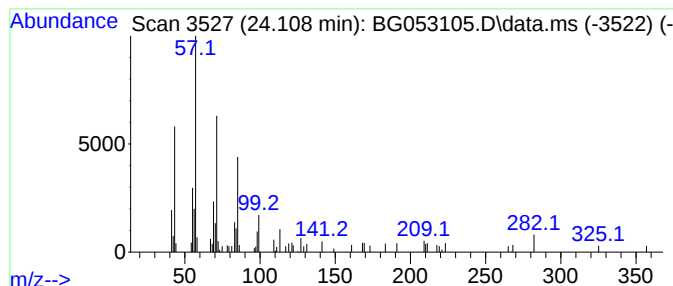
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.108	2.17 ng	67510	Perylene-d12	25.066

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	93
2			Nonadecane	268	C19H40	000629-92-5	87
3			Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	86
4			10-Methylnonadecane	282	C20H42	056862-62-5	86
5			Dodecane, 1-iodo-	296	C12H25I	004292-19-7	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041122\
Data File : BG053105.D
Acq On : 11 Apr 2022 17:35
Operator : CG/JU
Sample : N2317-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

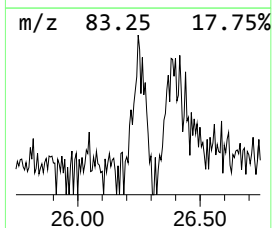
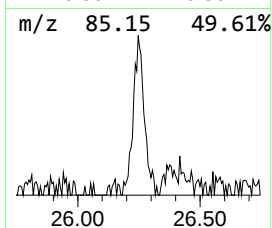
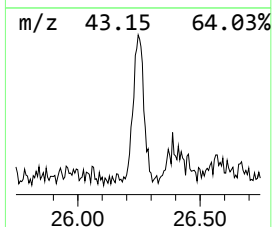
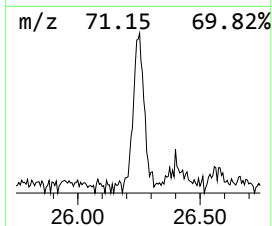
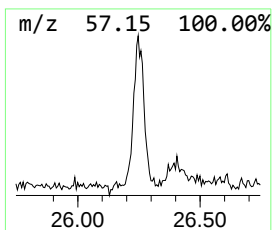
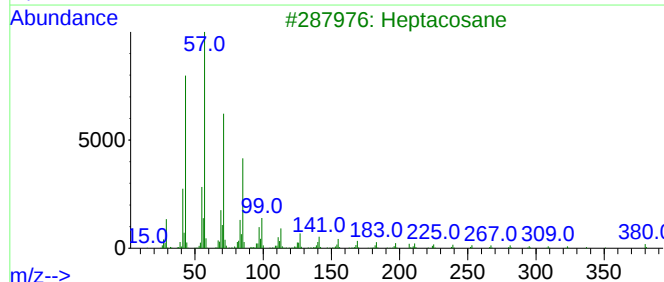
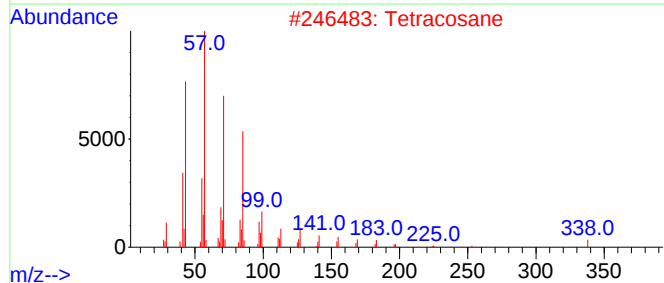
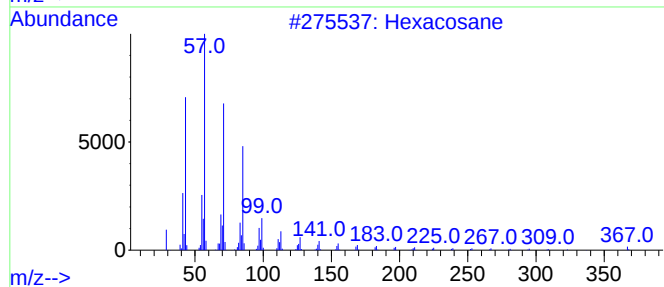
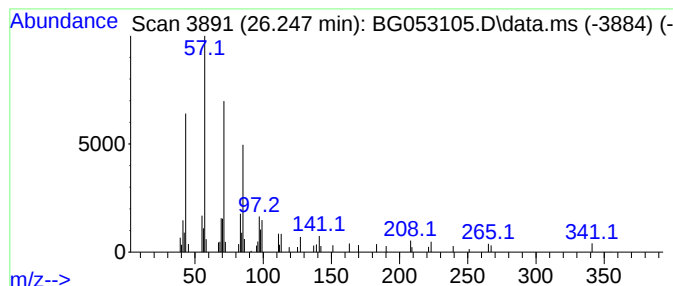
Instrument :
BNA_G
ClientSampleId :
NORTH-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
26.247	2.90 ng	90197	Perylene-d12	25.066	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	83
2	Tetracosane	338	C24H50	000646-31-1	83
3	Heptacosane	380	C27H56	000593-49-7	83
4	Heptadecane	240	C17H36	000629-78-7	80
5	Pentacosane	352	C25H52	000629-99-2	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041122\
Data File : BG053105.D
Acq On : 11 Apr 2022 17:35
Operator : CG/JU
Sample : N2317-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
NORTH-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.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-...	5.210	5.2	ng	47965	1	8.124	185113	20.0
Bicyclo[3.1.1]h...	6.808	5.9	ng	54380	1	8.124	185113	20.0
Cinnamyl cinnamate	21.212	24.4	ng	742639	5	21.764	609300	20.0
Trichloroacetic...	21.394	8.3	ng	253019	5	21.764	609300	20.0
Acetic acid, ch...	22.604	4.0	ng	120360	5	21.764	609300	20.0
Eicosane	24.108	2.2	ng	67510	6	25.066	622169	20.0
Hexacosane	26.247	2.9	ng	90197	6	25.066	622169	20.0