

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012623\
 Data File : BG056446.D
 Acq On : 26 Jan 2023 17:09
 Operator : CG/JU
 Sample : 01214-14
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 TJRC-011823-B3-30-40

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: BG056446.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.332	341	348	356	rBB	101180	156095	5.95%	1.528%
2	5.814	423	430	442	rBV	426699	679630	25.92%	6.655%
3	7.436	698	706	715	rBV	421188	726940	27.72%	7.118%
4	8.294	845	852	859	rBB	97467	162889	6.21%	1.595%
5	9.469	1044	1052	1064	rBB	242711	438690	16.73%	4.295%
6	11.126	1326	1334	1344	rBV	126394	229230	8.74%	2.245%
7	13.535	1737	1744	1754	rBV	1010600	1481855	56.52%	14.510%
8	14.909	1971	1978	1988	rBB	265242	406869	15.52%	3.984%
9	16.249	2200	2206	2212	rVB	30898	43982	1.68%	0.431%
10	16.390	2223	2230	2244	rBV	779037	1187351	45.28%	11.626%
11	17.647	2437	2444	2456	rVB	379732	566114	21.59%	5.543%
12	20.221	2876	2882	2889	rVB	2056412	2622018	100.00%	25.674%
13	20.879	2988	2994	2998	rBV6	25050	44393	1.69%	0.435%
14	21.513	3098	3102	3113	rBV3	49769	101065	3.85%	0.990%
15	21.778	3143	3147	3151	rVB	23030	33282	1.27%	0.326%
16	21.937	3168	3174	3181	rVB2	386150	644933	24.60%	6.315%
17	25.374	3747	3759	3771	rVB2	219922	687526	26.22%	6.732%

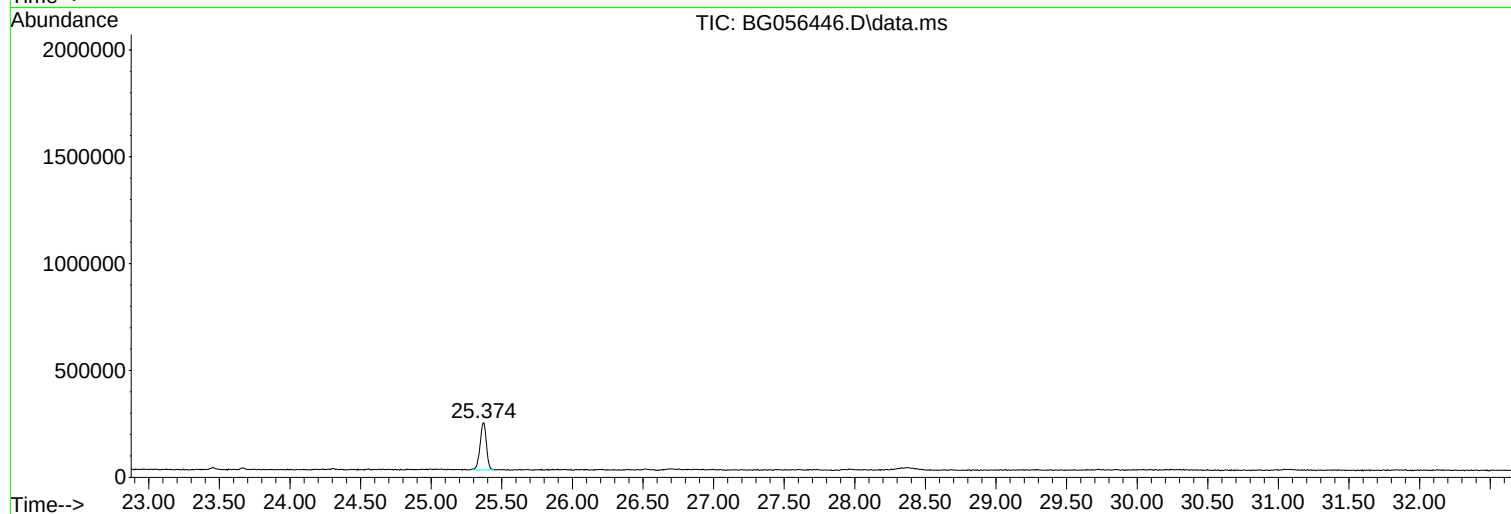
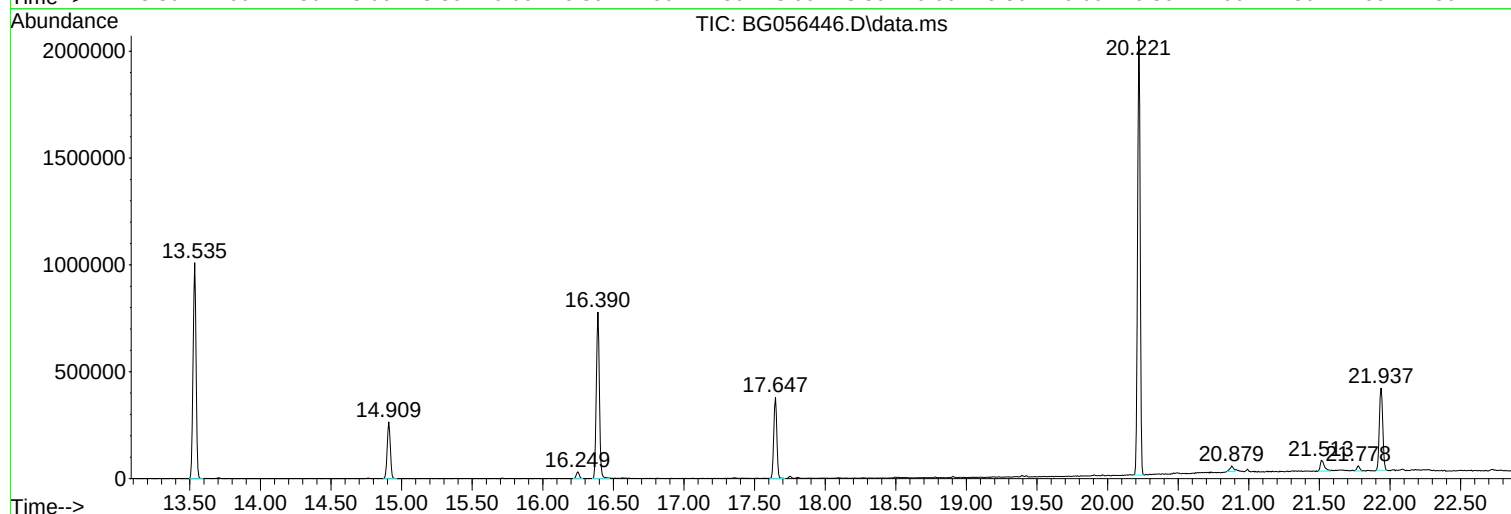
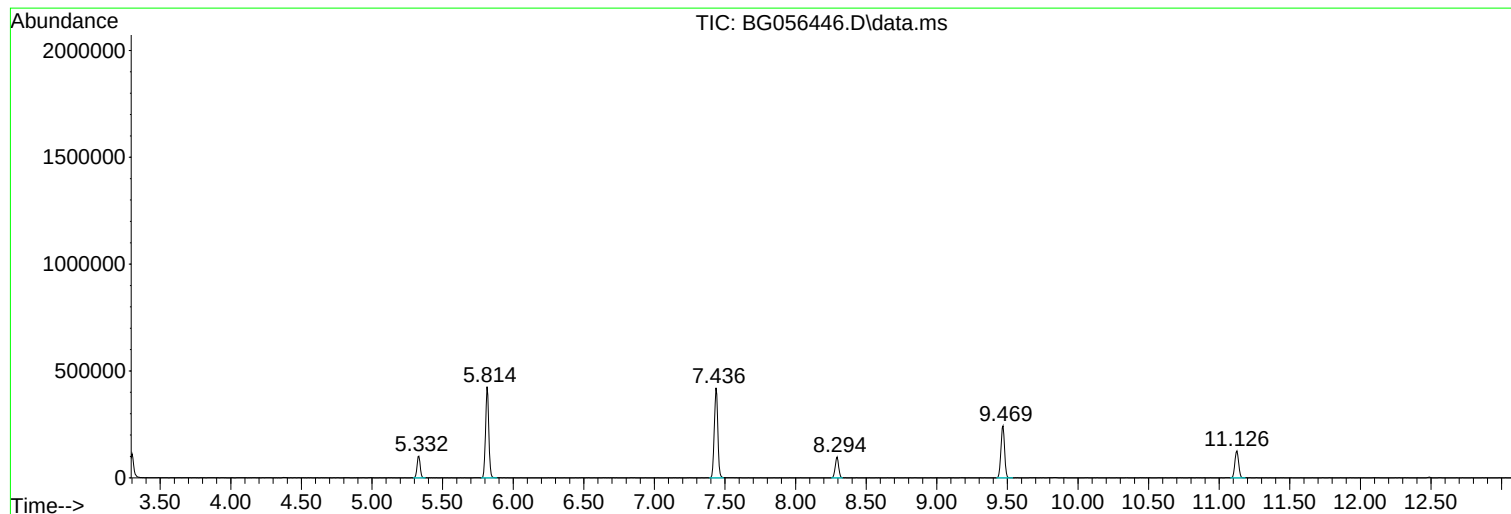
Sum of corrected areas: 10212862

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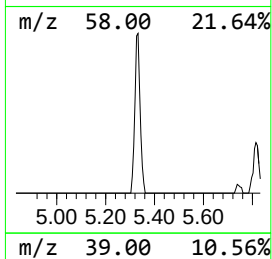
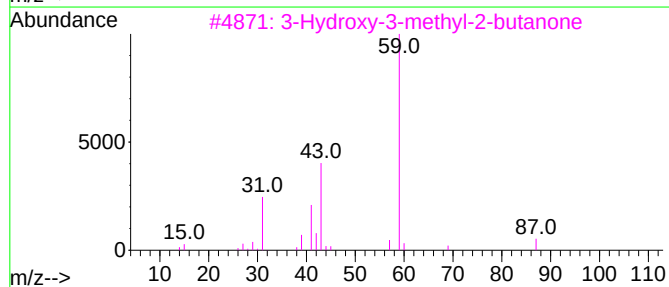
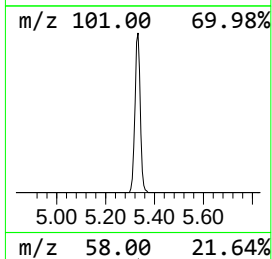
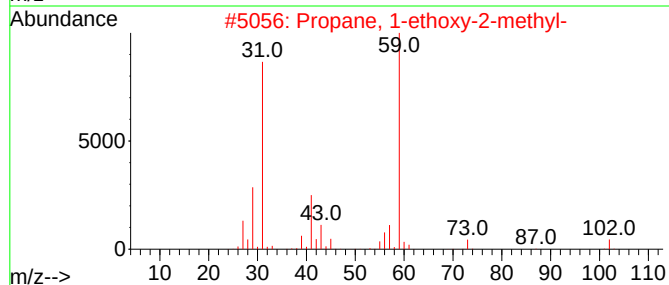
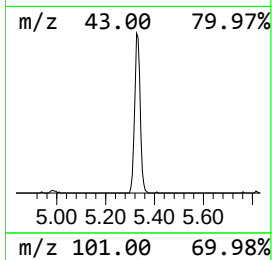
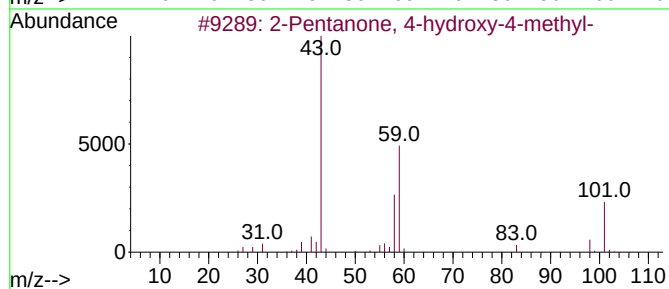
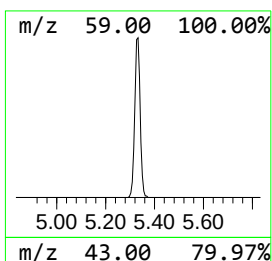
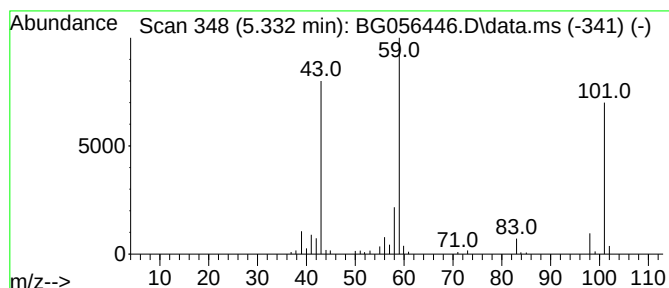
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.332	19.17 ng	156095	1,4-Dichlorobenzene-d4	8.294

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45	
2	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	35	
3	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	25	
4	4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	25	
5	1,2-Butanediol	90	C4H10O2	000584-03-2	23	



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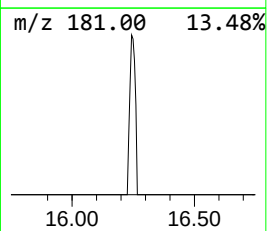
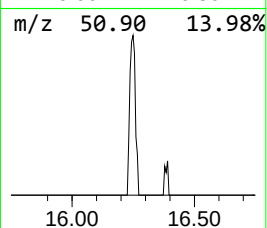
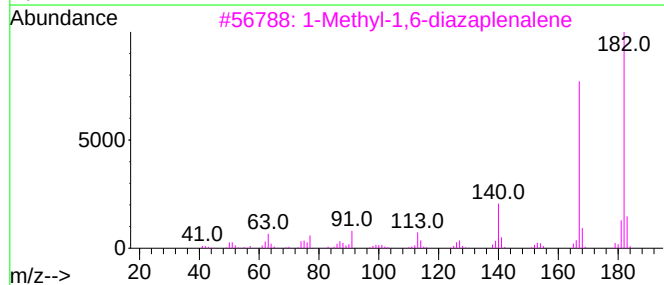
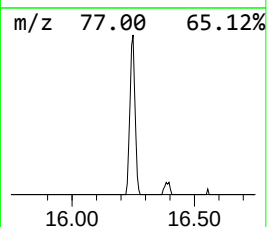
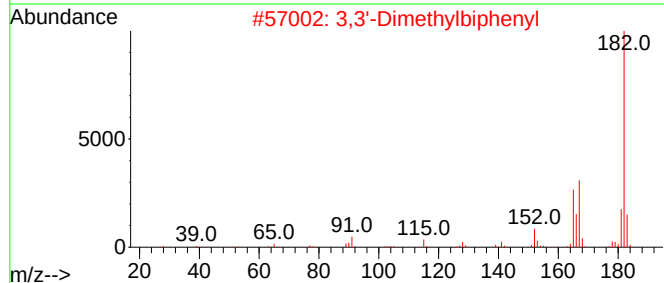
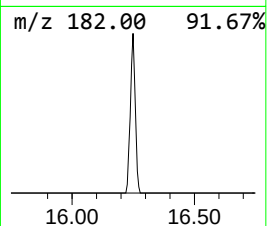
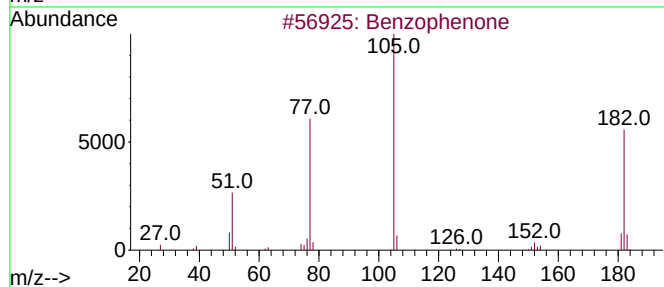
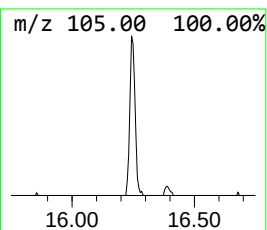
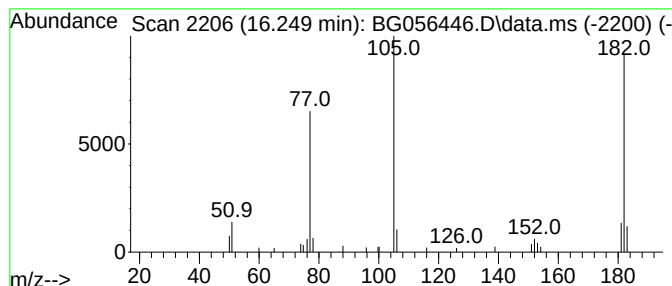
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Peak Number 2 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.249	2.16 ng	43982	Acenaphthene-d10	14.910

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	91
2			3,3'-Dimethylbiphenyl	182	C14H14	000612-75-9	43
3			1-Methyl-1,6-diazaplenalene	182	C12H10N2	079691-99-9	43
4			2-Methyl-1H-perimidine	182	C12H10N2	005157-10-8	38
5			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	27



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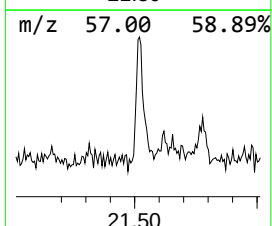
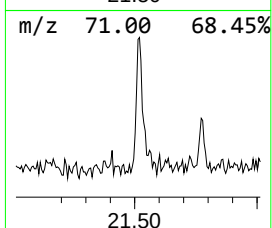
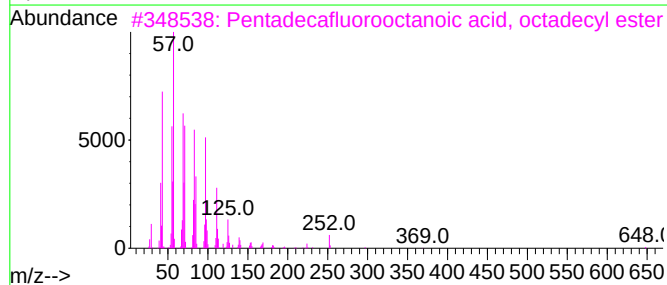
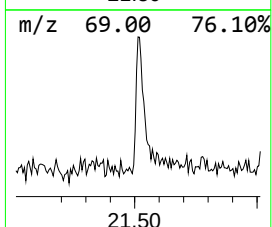
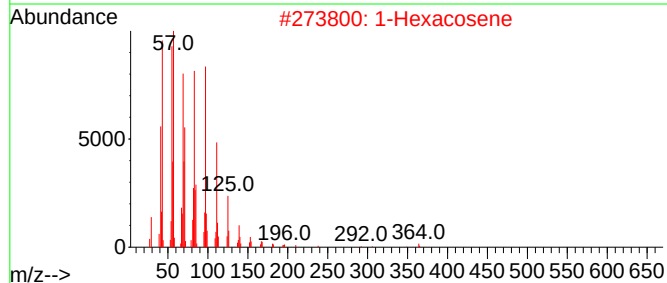
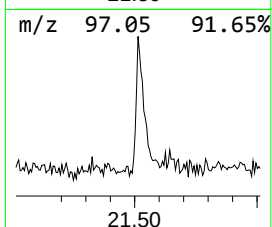
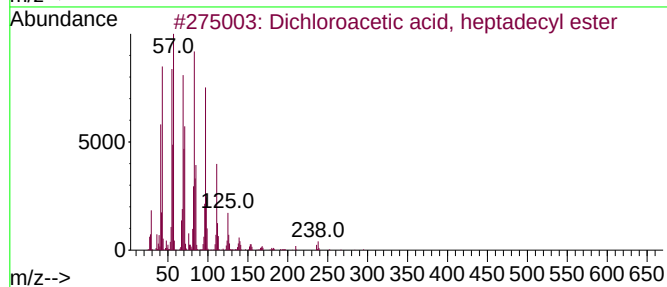
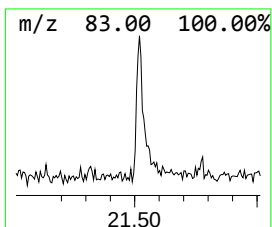
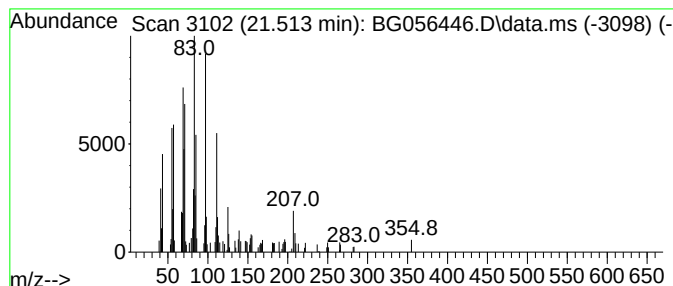
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Peak Number 3 Dichloroacetic acid, heptad... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.514	3.13 ng	101065	Chrysene-d12	21.936

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	86
2			1-Hexacosene	364	C26H52	018835-33-1	80
3			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	74
4			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	62
5			1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	62



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.332	19.2	ng	156095	1	8.294	162889	20.0
Benzophenone	16.249	2.2	ng	43982	3	14.910	406869	20.0
Dichloroacetic ...	21.514	3.1	ng	101065	5	21.936	644933	20.0