

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081221\
 Data File : BG049822.D
 Acq On : 12 Aug 2021 17:52
 Operator : CG/JU
 Sample : M3340-01
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 205-239-929

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-BG080321.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG049822.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.139	12	17	22	rBV	68451	109340	5.90%	0.947%
2	5.113	347	353	363	rVB2	31664	55158	2.98%	0.478%
3	5.589	427	434	446	rBV	567934	937834	50.58%	8.125%
4	7.199	699	708	718	rBV	598455	1072783	57.86%	9.294%
5	8.033	840	850	858	rBV	139678	239788	12.93%	2.077%
6	9.208	1041	1050	1059	rBV	384228	709224	38.25%	6.145%
7	10.617	1283	1290	1302	rBV3	23441	49512	2.67%	0.429%
8	10.858	1322	1331	1338	rBV	185186	341277	18.41%	2.957%
9	13.308	1740	1748	1755	rBV	1033564	1611650	86.93%	13.963%
10	14.688	1974	1983	1990	rBV	295799	466199	25.15%	4.039%
11	16.181	2231	2237	2245	rBV	846818	1275453	68.79%	11.050%
12	16.421	2274	2278	2282	rVB4	13412	20585	1.11%	0.178%
13	16.510	2286	2293	2296	rBV2	21783	34802	1.88%	0.302%
14	16.568	2298	2303	2309	rVV4	16667	38331	2.07%	0.332%
15	16.633	2309	2314	2318	rVV3	20249	33486	1.81%	0.290%
16	16.674	2318	2321	2326	rVB4	12689	19141	1.03%	0.166%
17	16.833	2343	2348	2355	rVB6	21954	40273	2.17%	0.349%
18	16.897	2355	2359	2363	rBV	22074	32055	1.73%	0.278%
19	16.974	2368	2372	2375	rVB4	12858	19442	1.05%	0.168%
20	17.444	2445	2452	2456	rBV	322709	507014	27.35%	4.393%
21	17.485	2456	2459	2466	rVB	54591	78881	4.25%	0.683%
22	18.319	2596	2601	2606	rBV3	55078	85292	4.60%	0.739%
23	18.366	2606	2609	2616	rVB2	24917	42598	2.30%	0.369%
24	18.513	2630	2634	2638	rBV3	21010	36768	1.98%	0.319%
25	18.548	2638	2640	2646	rVB2	18620	25021	1.35%	0.217%
26	18.613	2646	2651	2656	rBV8	11753	23704	1.28%	0.205%
27	18.818	2681	2686	2689	rBV5	13653	21676	1.17%	0.188%
28	18.859	2690	2693	2698	rVB7	14008	23656	1.28%	0.205%
29	19.229	2753	2756	2761	rBV3	29553	46209	2.49%	0.400%
30	19.382	2776	2782	2786	rBV8	19028	45474	2.45%	0.394%
31	19.494	2796	2801	2807	rVB	122883	181451	9.79%	1.572%
32	19.858	2859	2863	2870	rVB2	172995	256809	13.85%	2.225%
33	19.923	2872	2874	2882	rVB9	15310	24158	1.30%	0.209%
34	20.052	2890	2896	2901	rBV	1440773	1854031	100.00%	16.063%
35	20.510	2971	2974	2978	rVB2	27646	30768	1.66%	0.267%
36	20.645	2995	2997	3001	rBV	21735	26759	1.44%	0.232%

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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-BG080321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	20.733	3010	3012	3018	rVB2	37262	39031	2.11%	0.338%
38	21.350	3114	3117	3122	rBV5	38982	52448	2.83%	0.454%
39	21.591	3155	3158	3163	rVB2	39698	63236	3.41%	0.548%
40	21.726	3174	3181	3186	rBV2	281779	521410	28.12%	4.517%
41	23.958	3557	3561	3562	rBV4	34360	46033	2.48%	0.399%
42	25.010	3733	3740	3752	rVB2	147235	403580	21.77%	3.497%

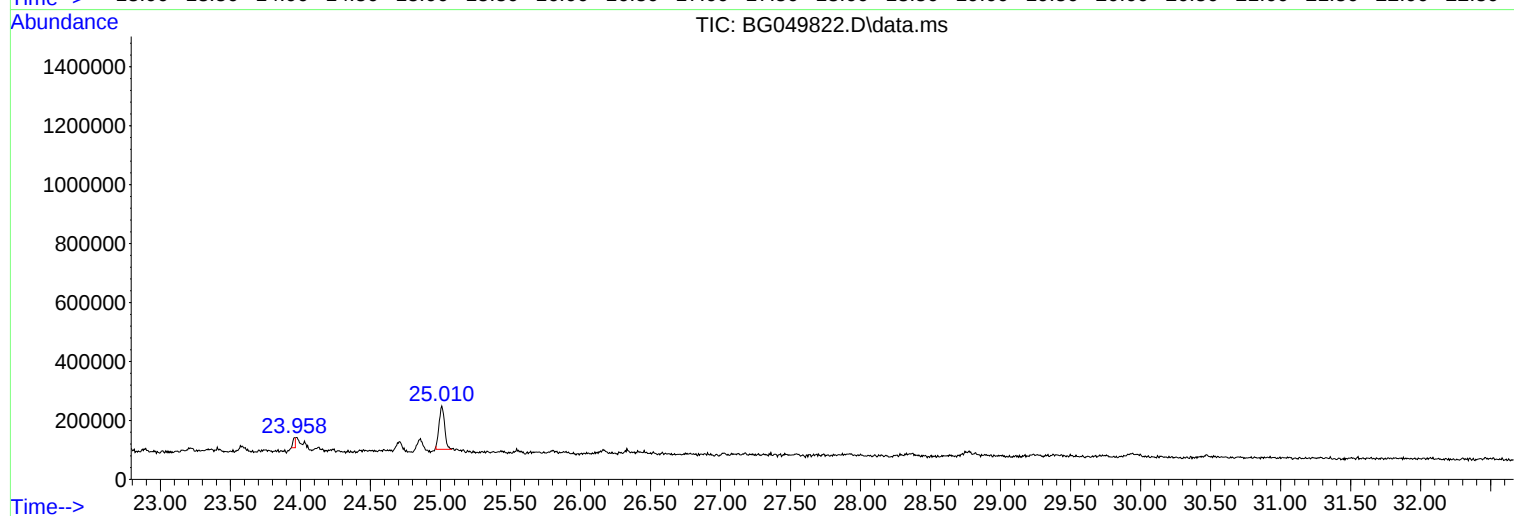
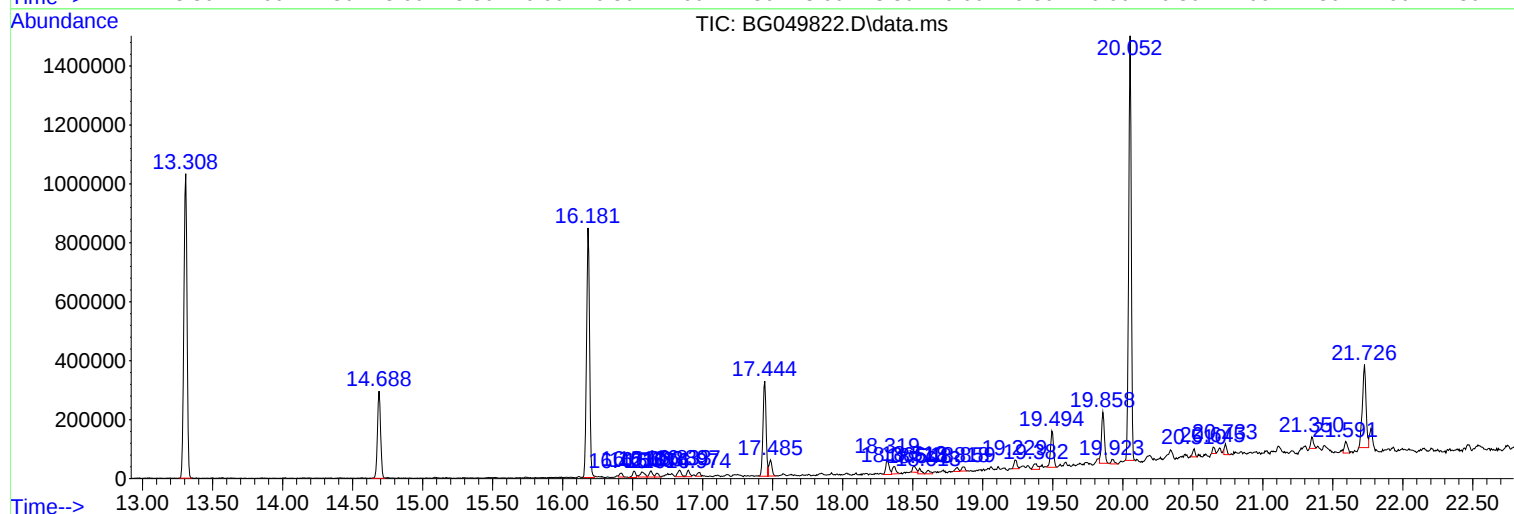
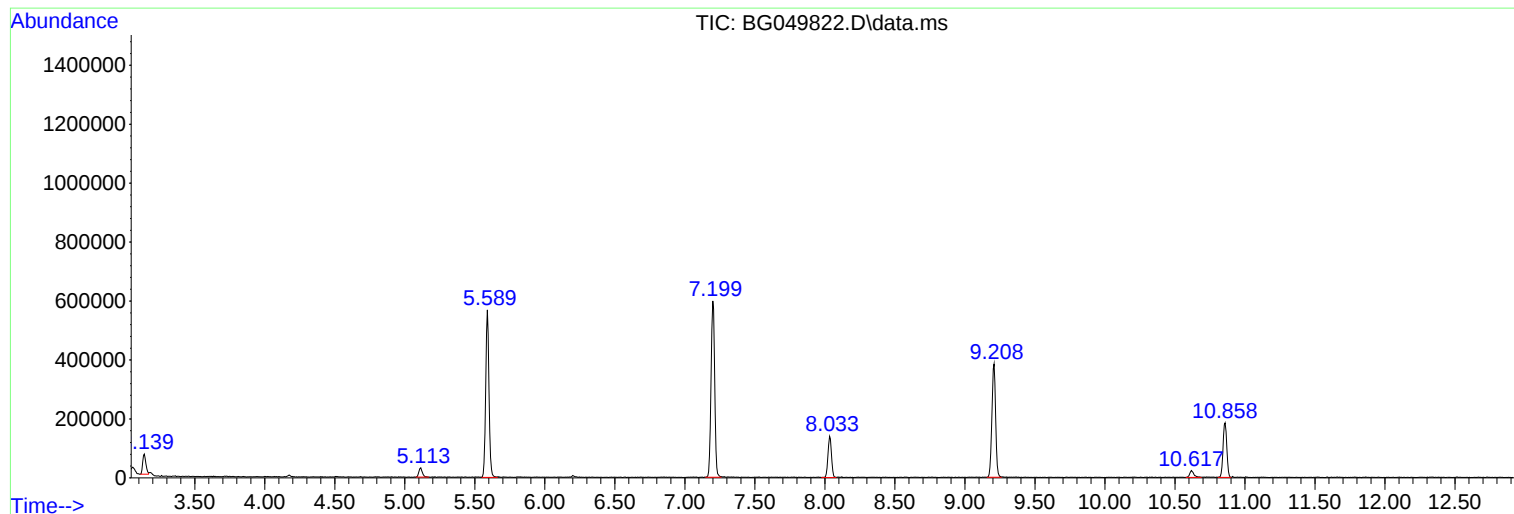
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Instrument :
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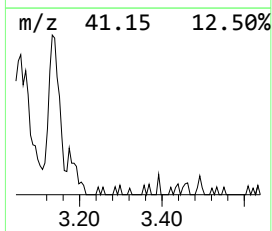
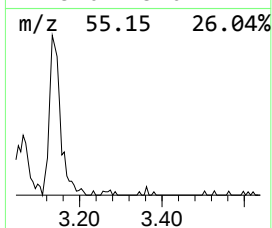
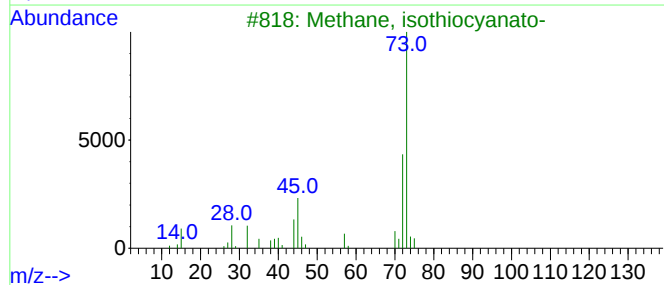
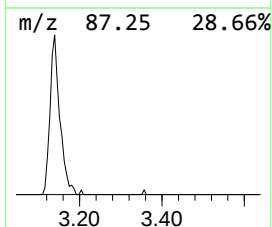
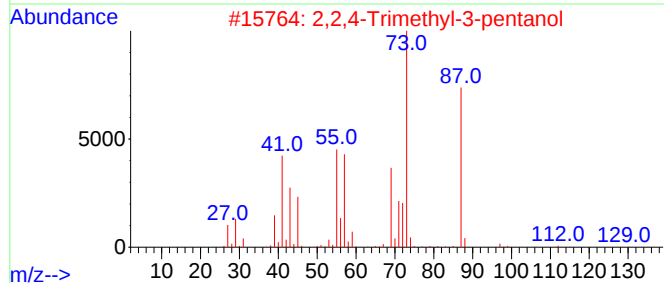
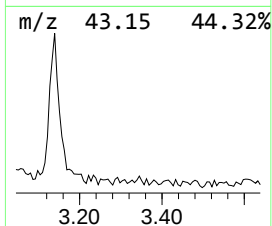
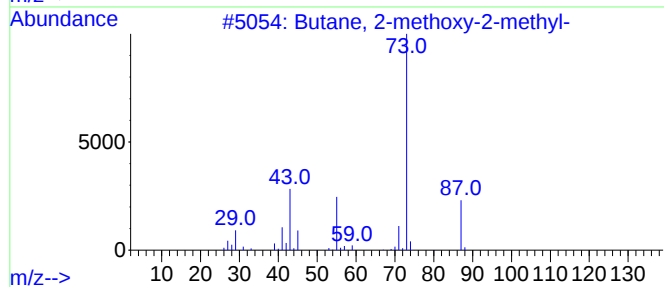
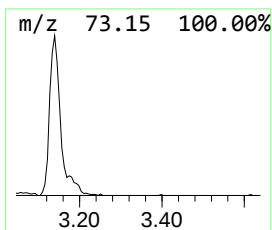
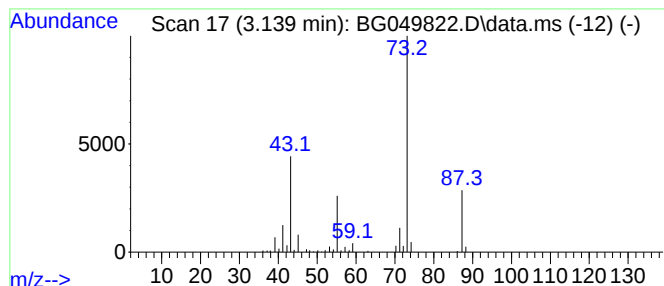
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.139	9.12 ng	109340	1,4-Dichlorobenzene-d4	8.033

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	64
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	36
3			Methane, isothiocyanato-	73	C2H3NS	000556-61-6	9
4			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	9
5			Silane, ethyltrimethyl-	102	C5H14Si	003439-38-1	9



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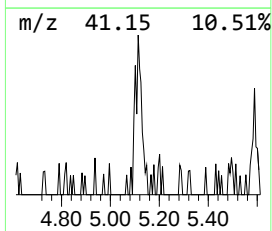
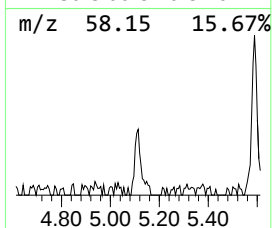
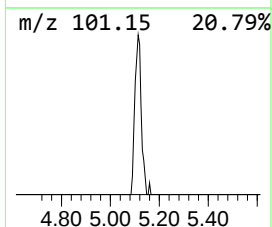
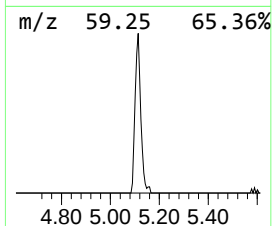
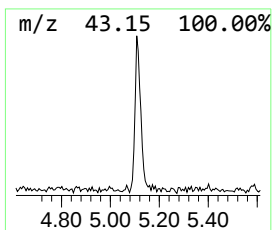
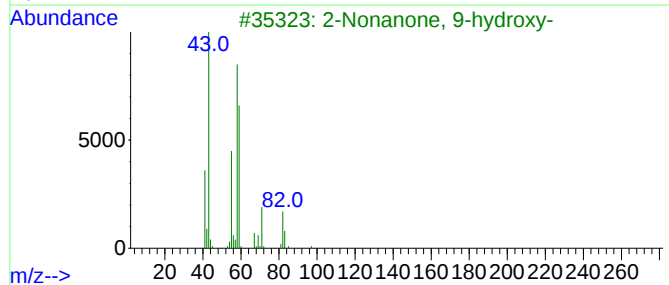
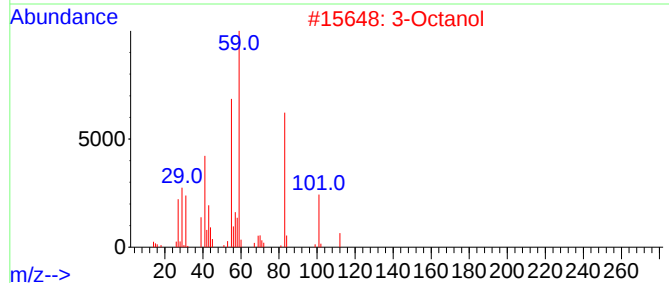
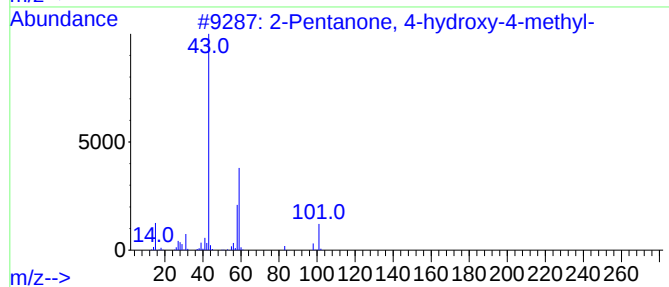
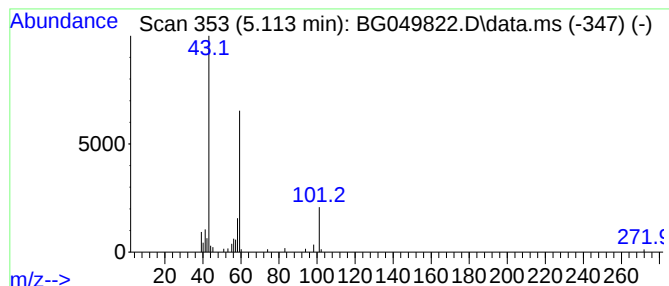
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.113	4.60 ng	55158	1,4-Dichlorobenzene-d4	8.033

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	42
2			3-Octanol	130	C8H18O	000589-98-0	33
3			2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	28
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
5			1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	25



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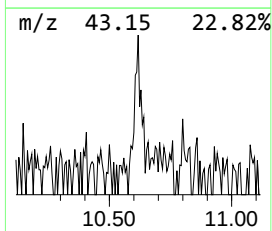
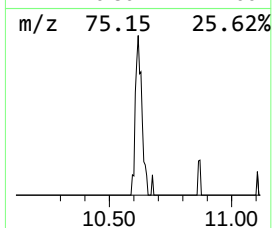
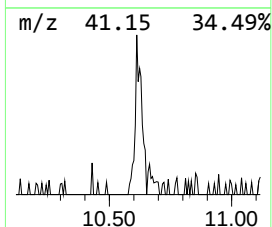
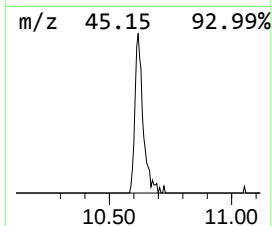
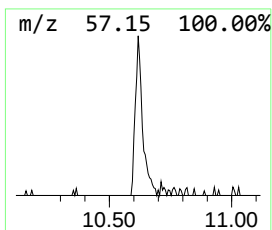
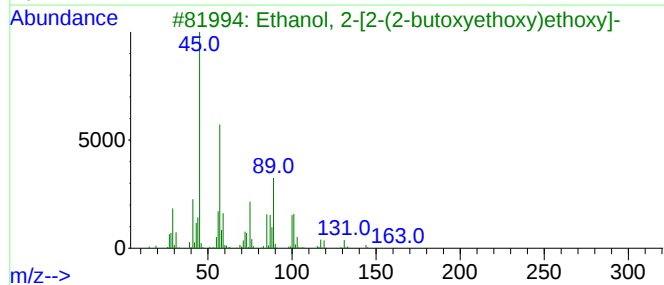
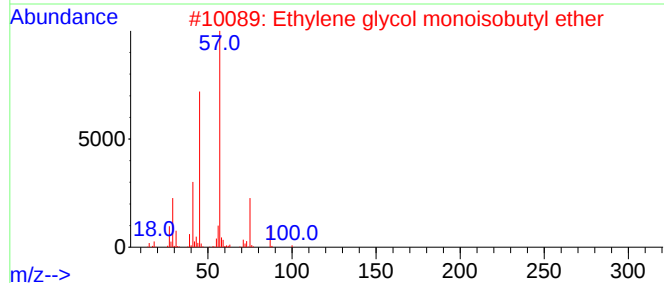
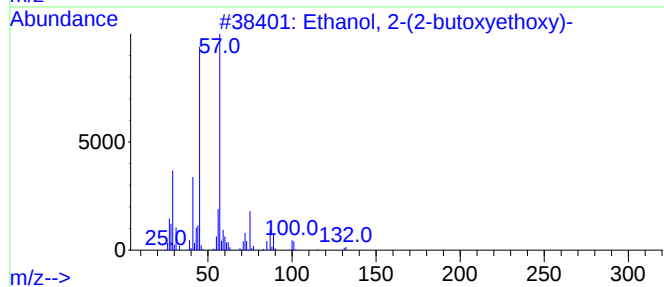
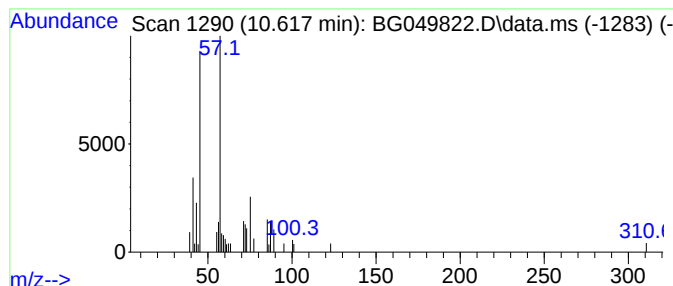
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.618	2.90 ng	49512	Naphthalene-d8	10.858

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	64
2			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	59
3			Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	45
4			Propanoic acid, 2-(methoxymethoxy)-	134	C5H10O4	081327-29-9	43
5			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	43



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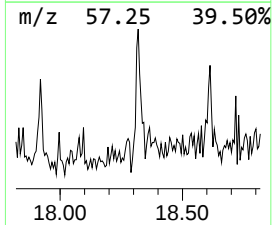
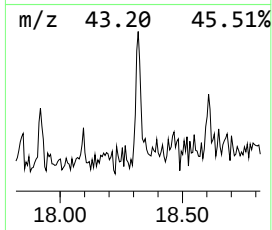
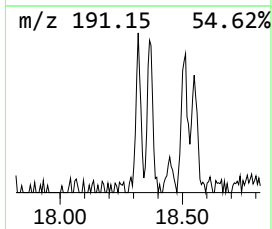
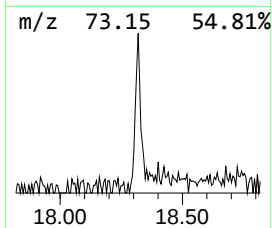
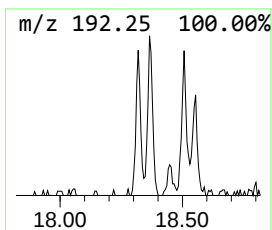
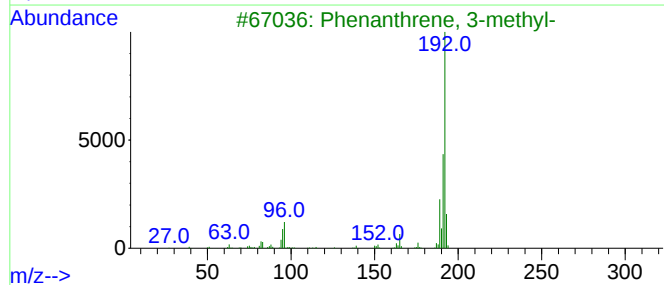
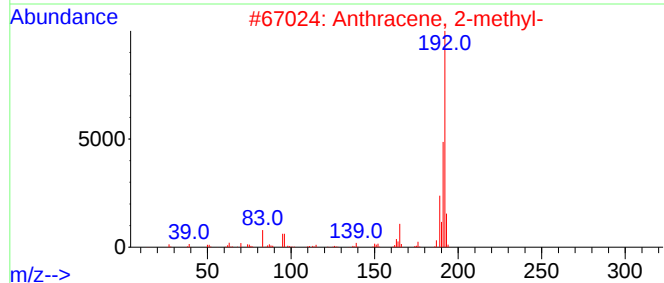
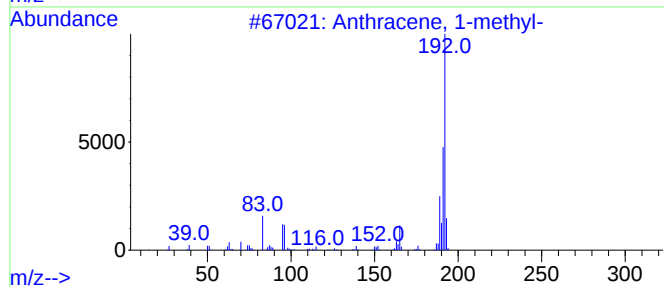
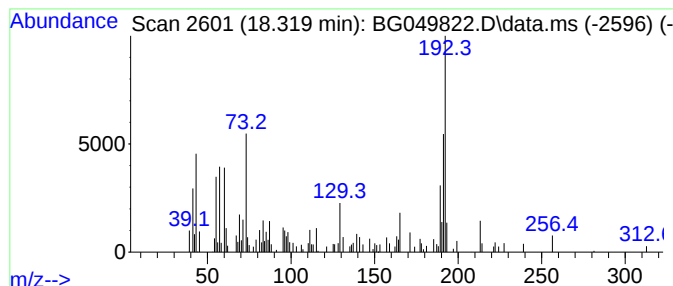
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Anthracene, 1-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.319	3.36 ng	85292	Phenanthrene-d10	17.444

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Anthracene, 1-methyl-	192	C15H12	000610-48-0	90
2		Anthracene, 2-methyl-	192	C15H12	000613-12-7	70
3		Phenanthrene, 3-methyl-	192	C15H12	000832-71-3	70
4		Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	55
5		Anthracene, 9-methyl-	192	C15H12	000779-02-2	55



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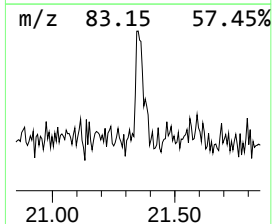
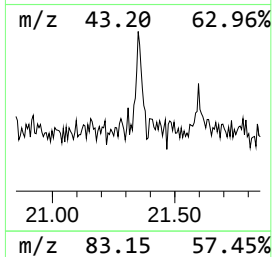
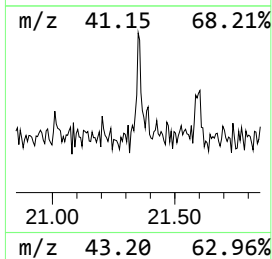
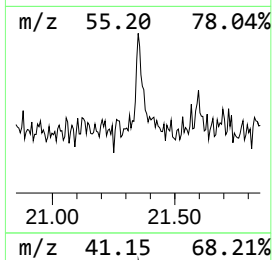
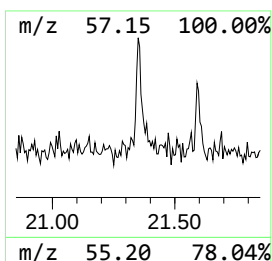
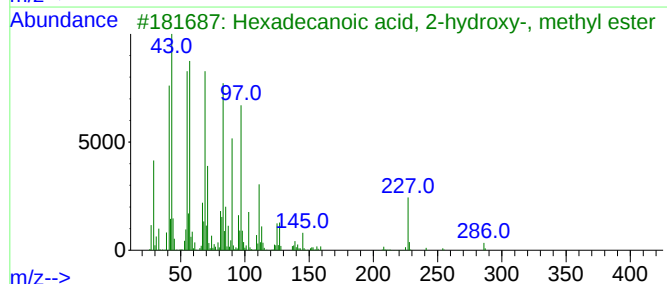
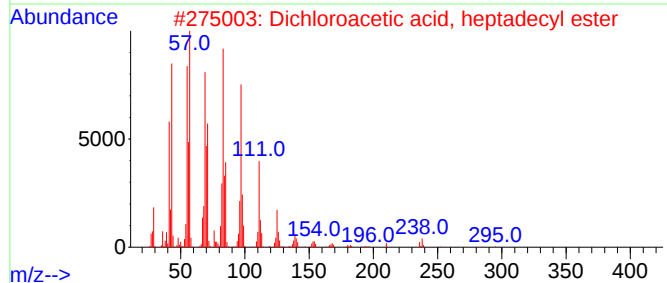
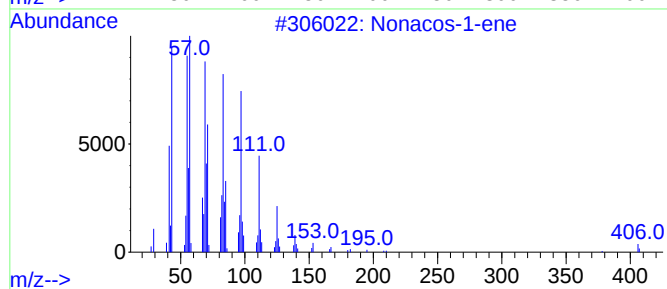
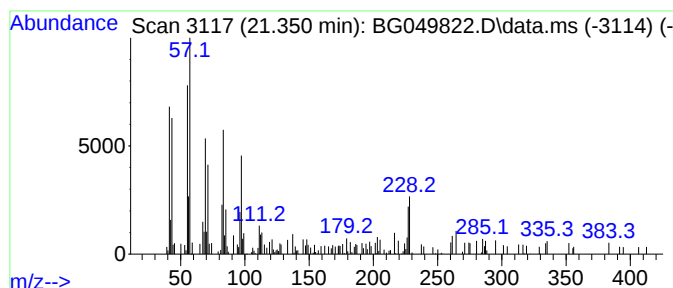
Instrument :
BNA_G
ClientSampleId :
205-239-929

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Nonacos-1-ene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.350	2.01 ng	52448	Chrysene-d12	21.726	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonacos-1-ene	406	C29H58	018835-35-3	64
2	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	52
3	Hexadecanoic acid, 2-hydroxy-, m...	286	C17H34O3	016742-51-1	49
4	Cyclohexane, (1-hexyltetradecyl)-	364	C26H52	004443-60-1	46
5	1-Hexacosanol	382	C26H54O	000506-52-5	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081221\
Data File : BG049822.D
Acq On : 12 Aug 2021 17:52
Operator : CG/JU
Sample : M3340-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
205-239-929

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	3.139	9.1	ng	109340	1	8.033	239788	20.0
2-Pentanone, 4-...	5.113	4.6	ng	55158	1	8.033	239788	20.0
Ethanol, 2-(2-b...	10.618	2.9	ng	49512	2	10.858	341277	20.0
Anthracene, 1-m...	18.319	3.4	ng	85292	4	17.444	507014	20.0
Nonacos-1-ene	21.350	2.0	ng	52448	5	21.726	521410	20.0