

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081621\
 Data File : BG049862.D
 Acq On : 16 Aug 2021 23:13
 Operator : CG/JU
 Sample : M3404-04
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 TP2-1-6FT

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: BG049862.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.141	11	17	24	rBV	95613	176593	8.52%	1.354%
2	5.109	347	352	360	rBV	56344	94176	4.54%	0.722%
3	5.584	427	433	444	rBV	639654	1076118	51.89%	8.252%
4	7.200	699	708	718	rBV	672781	1208106	58.26%	9.264%
5	8.028	841	849	857	rBV	130951	221396	10.68%	1.698%
6	9.203	1041	1049	1056	rBV	436095	801247	38.64%	6.144%
7	10.607	1281	1288	1301	rBV	102911	194669	9.39%	1.493%
8	10.848	1322	1329	1337	rBV	164256	305240	14.72%	2.341%
9	13.298	1736	1746	1754	rBV	1083834	1739881	83.90%	13.341%
10	14.678	1974	1981	1988	rBV	249677	406724	19.61%	3.119%
11	16.176	2230	2236	2247	rBV	906997	1387448	66.90%	10.639%
12	17.433	2444	2450	2455	rBV	292398	456488	22.01%	3.500%
13	17.474	2455	2457	2464	rVV	58681	78583	3.79%	0.603%
14	18.085	2557	2561	2565	rVB	27428	31586	1.52%	0.242%
15	18.308	2594	2599	2603	rBV3	20116	31172	1.50%	0.239%
16	18.361	2603	2608	2614	rVB3	22658	36398	1.76%	0.279%
17	18.502	2627	2632	2636	rBV3	19655	37730	1.82%	0.289%
18	18.543	2636	2639	2645	rVB3	12815	21252	1.02%	0.163%
19	19.225	2748	2755	2758	rBV5	18818	34923	1.68%	0.268%
20	19.366	2775	2779	2786	rBV6	12951	24085	1.16%	0.185%
21	19.489	2794	2800	2806	rVB	191494	273922	13.21%	2.100%
22	19.818	2851	2856	2857	rBV3	32043	42181	2.03%	0.323%
23	19.848	2857	2861	2868	rVB	155135	251703	12.14%	1.930%
24	19.918	2869	2873	2878	rVB6	14120	23019	1.11%	0.177%
25	20.047	2888	2895	2900	rBV	1587325	2073803	100.00%	15.902%
26	20.341	2941	2945	2949	rVB3	31398	46391	2.24%	0.356%
27	20.500	2967	2972	2975	rVV4	14186	21908	1.06%	0.168%
28	21.105	3071	3075	3079	rBV	18950	26017	1.25%	0.199%
29	21.293	3102	3107	3111	rBV5	14722	27417	1.32%	0.210%
30	21.340	3111	3115	3120	rBV4	45976	73196	3.53%	0.561%
31	21.439	3128	3132	3134	rBV5	13930	20880	1.01%	0.160%
32	21.716	3171	3179	3184	rBV2	278067	605563	29.20%	4.643%
33	21.763	3184	3187	3192	rVB	80947	122450	5.90%	0.939%
34	22.532	3312	3318	3326	rVB	14675	40778	1.97%	0.313%
35	23.948	3552	3559	3560	rBV	62856	105924	5.11%	0.812%
36	24.682	3678	3684	3694	rVB	43919	115285	5.56%	0.884%

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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	24.829	3700	3709	3719	rBV2	56259	183101	8.83%	1.404%
38	24.994	3726	3737	3746	rBV2	156341	486936	23.48%	3.734%
39	28.718	4365	4371	4381	rBV5	21529	75182	3.63%	0.576%
40	29.905	4567	4573	4582	rVB3	20400	61917	2.99%	0.475%

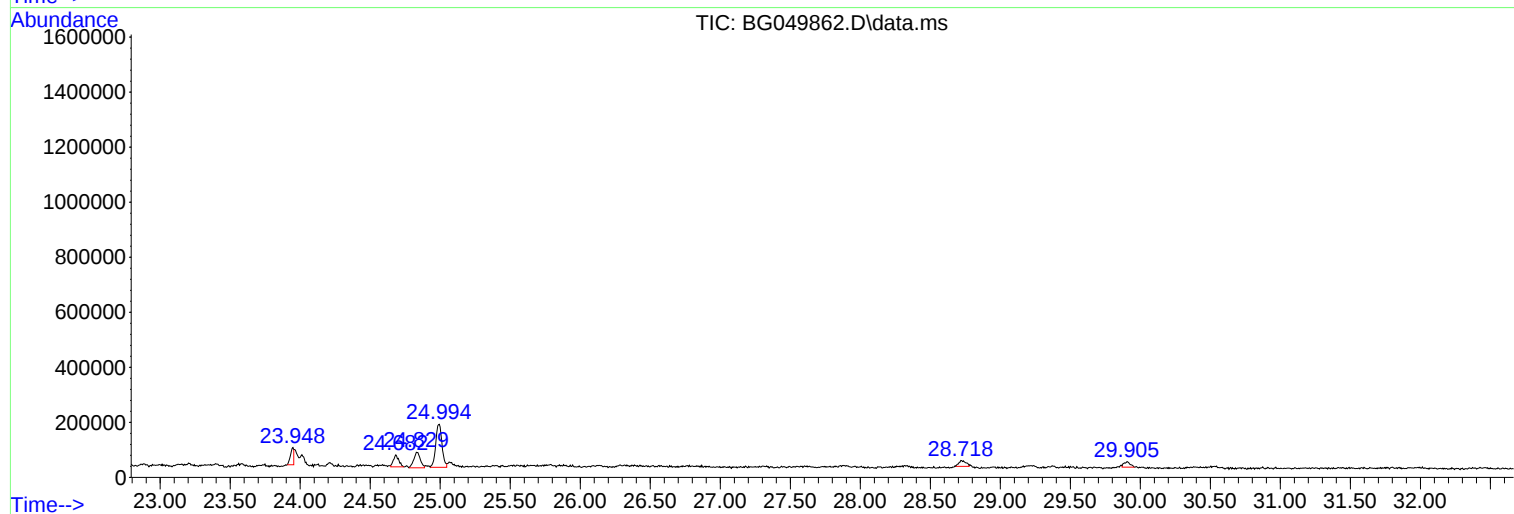
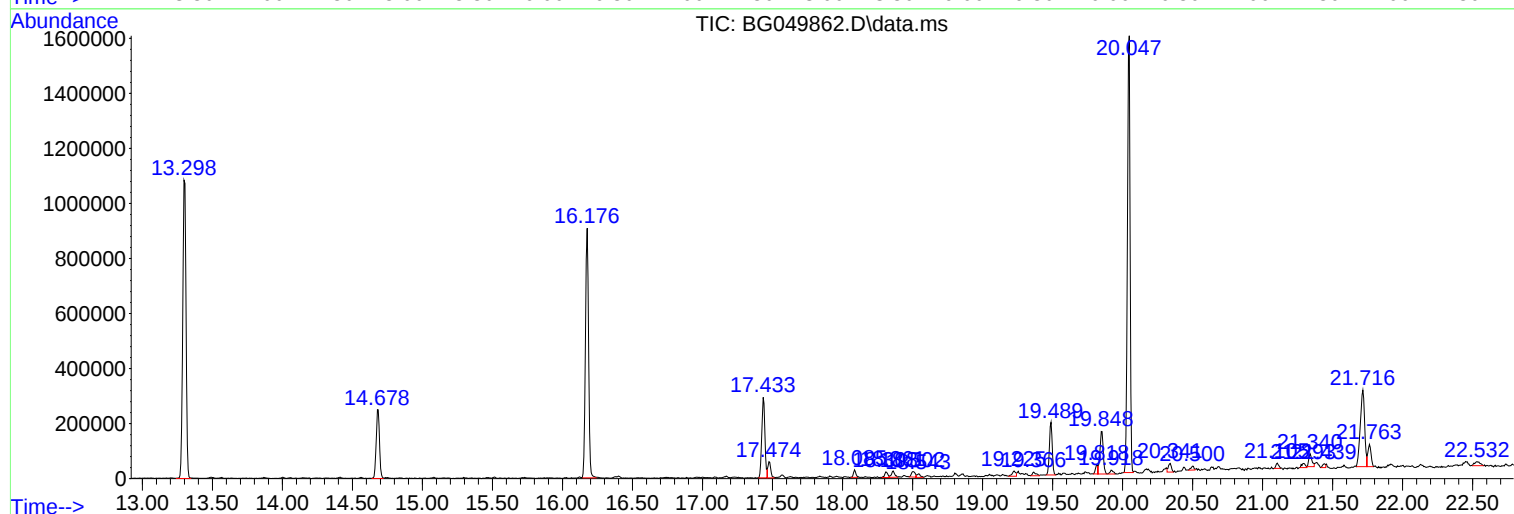
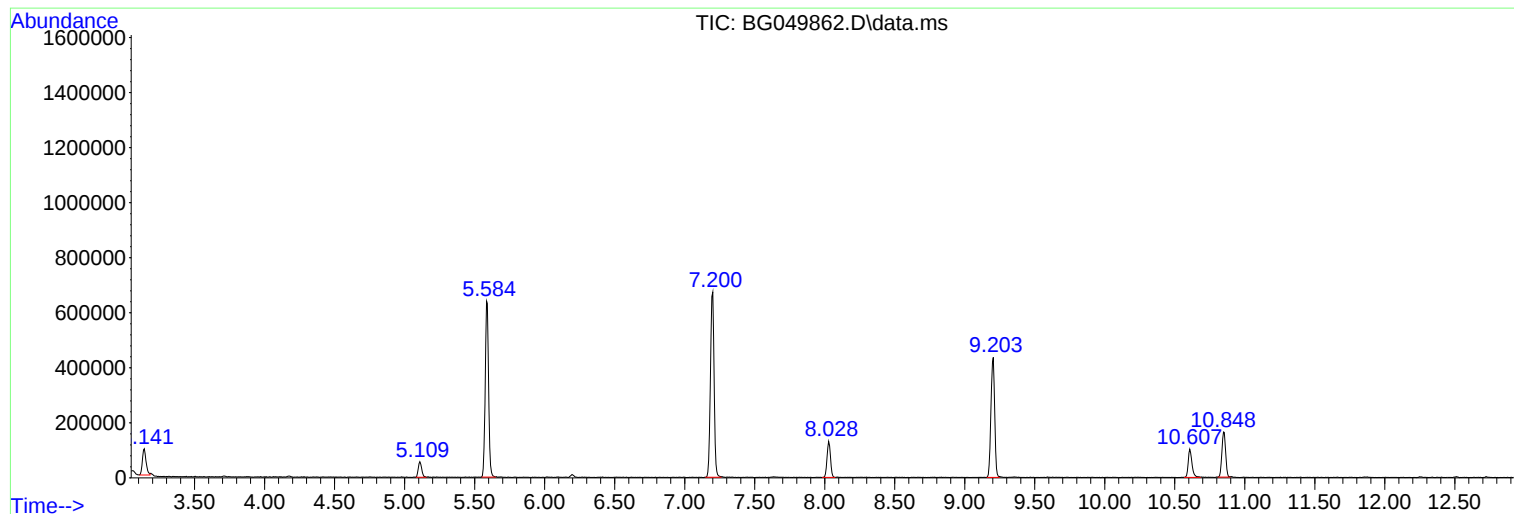
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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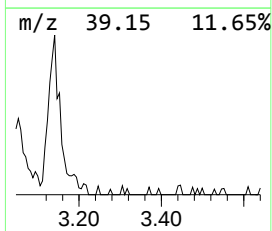
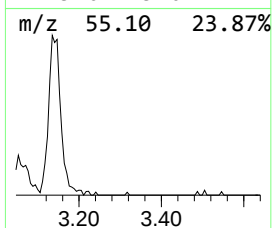
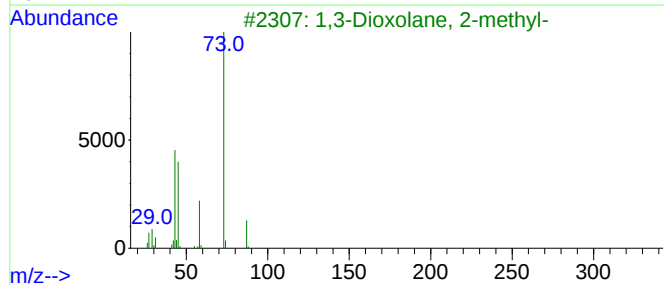
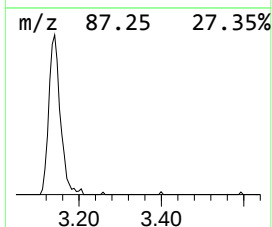
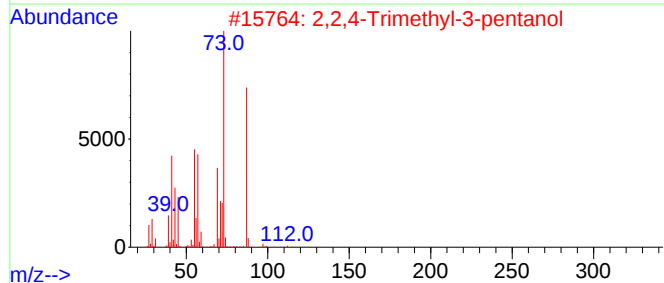
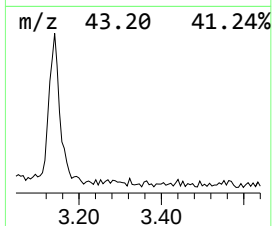
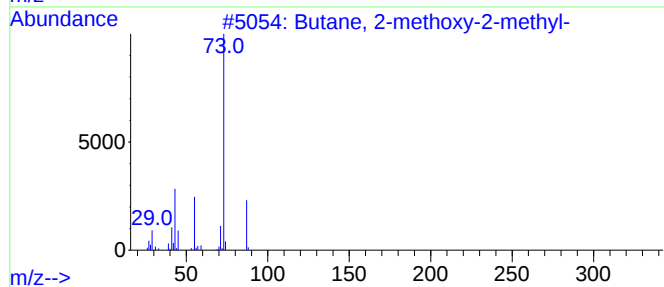
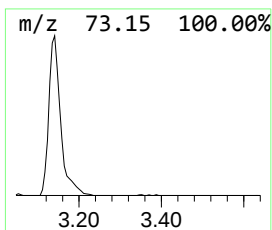
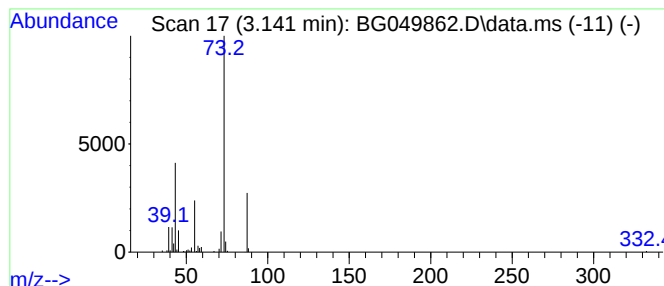
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
3.141	15.95 ng	176593	1,4-Dichlorobenzene-d4	8.028

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	38
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
5			N-Ethylformamide	73	C3H7NO	000627-45-2	9



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Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP2-1-6FT

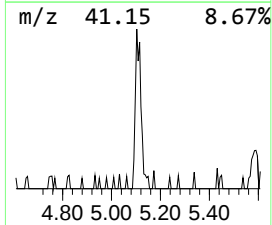
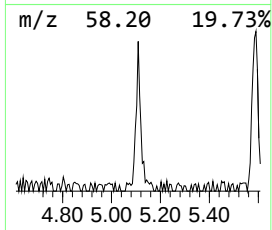
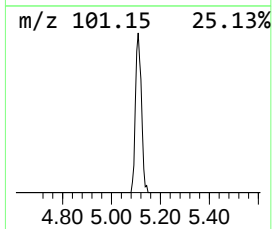
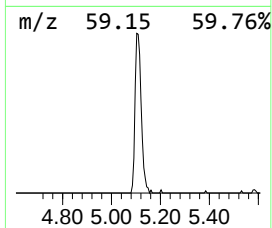
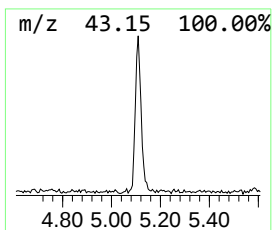
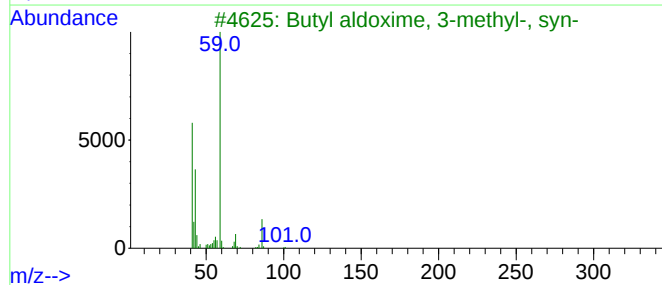
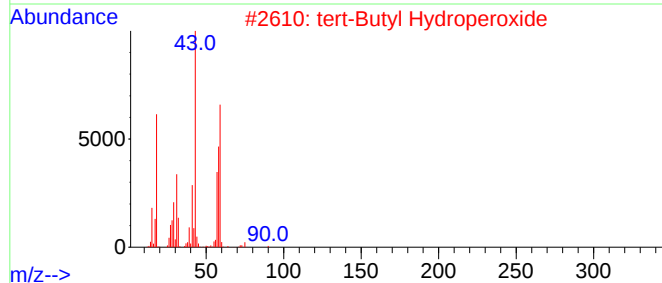
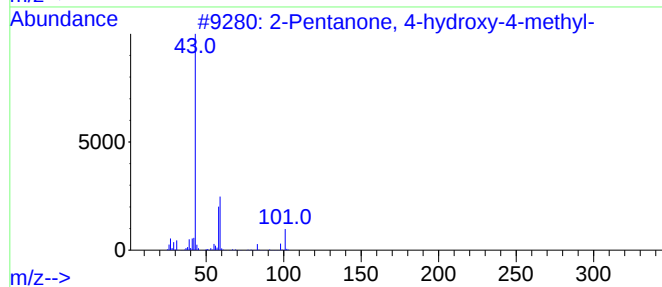
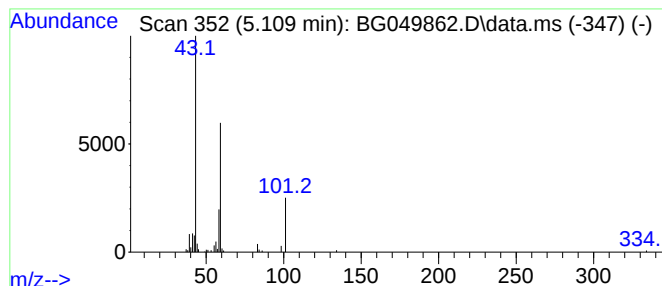
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.109	8.51 ng	94176	1,4-Dichlorobenzene-d4	8.028

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2			tert-Butyl Hydroperoxide	90	C4H10O2	000075-91-2	23
3			Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	12
4			1-Butene, 4-ethoxy-	100	C6H12O	044611-46-3	12
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	12



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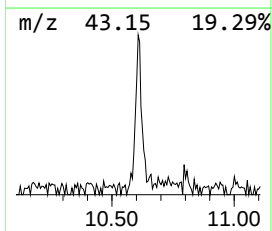
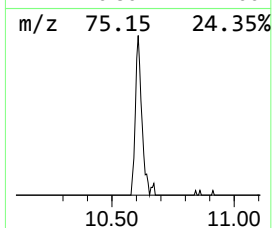
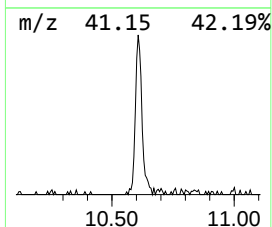
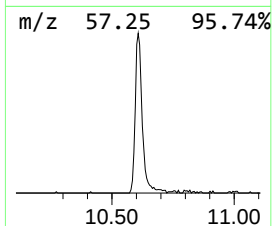
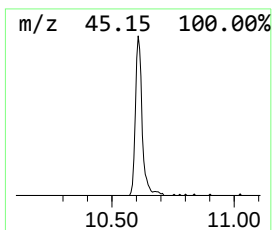
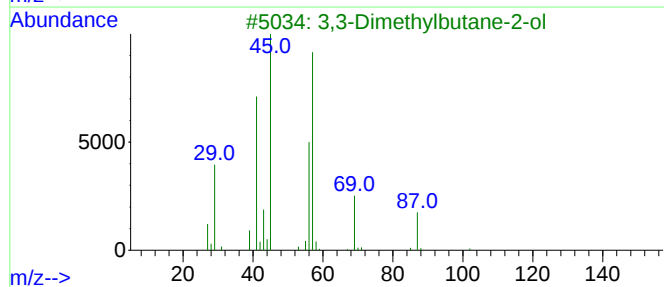
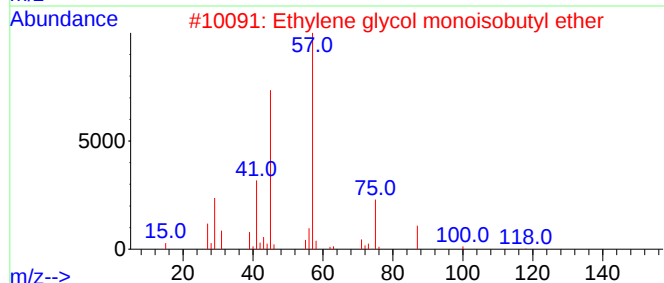
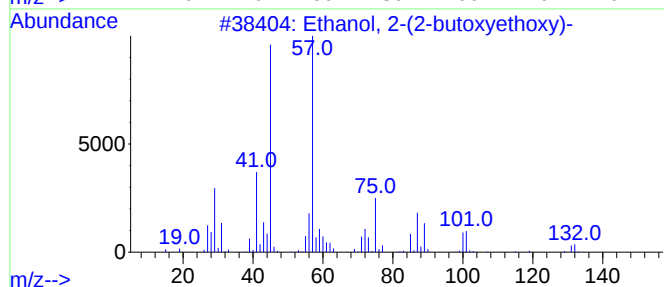
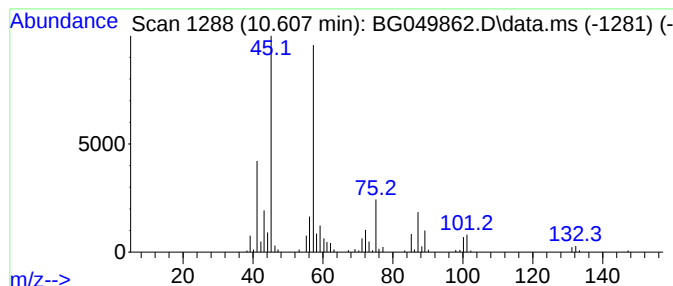
Instrument :
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.607	12.76 ng	194669	Naphthalene-d8	10.854	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	91
2	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	59
3	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	50
4	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	50
5	Methoxyacetic acid, 2-butyl ester	146	C7H14O3	070159-90-9	47



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ClientSampleId :
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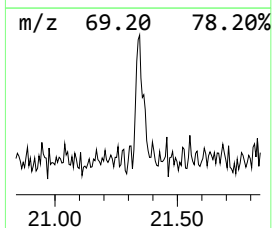
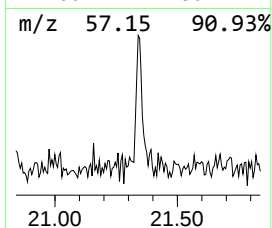
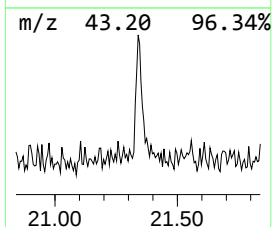
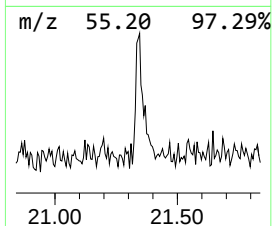
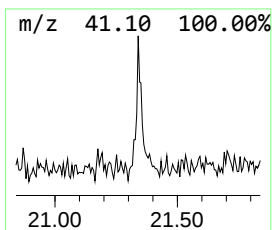
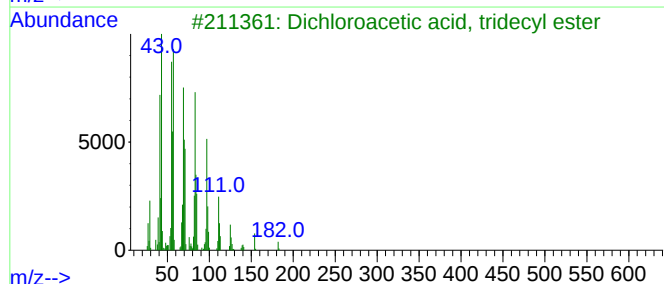
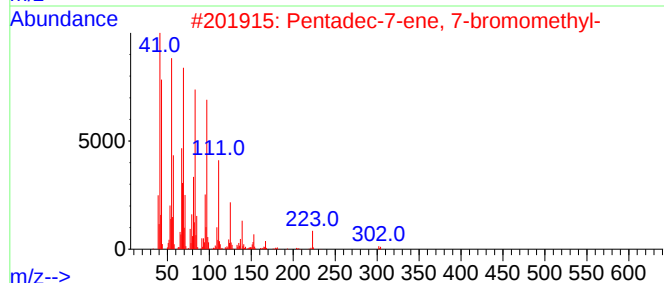
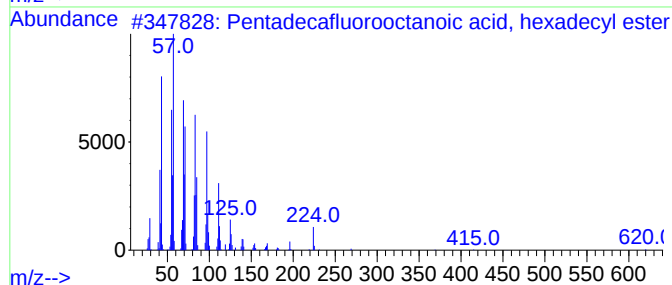
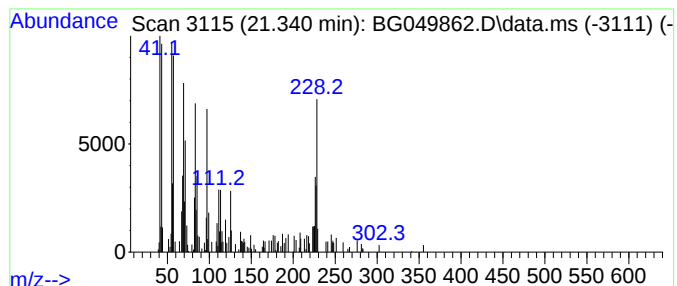
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 unknown21.340 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.340	2.42 ng	73196	Chrysene-d12	21.716

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecafluorooctanoic acid, he...	638	C24H33F15O2	1000406-04-6	46
2			Pentadec-7-ene, 7-bromomethyl-	302	C16H31Br	1000259-58-5	46
3			Dichloroacetic acid, tridecyl ester	310	C15H28Cl2O2	1000280-48-3	43
4			1-Tridecene	182	C13H26	002437-56-1	41
5			Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	25



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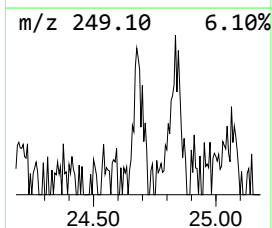
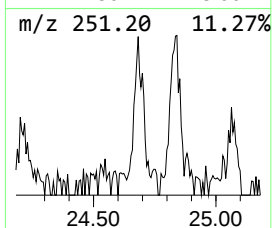
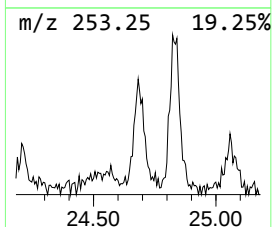
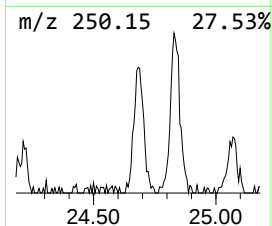
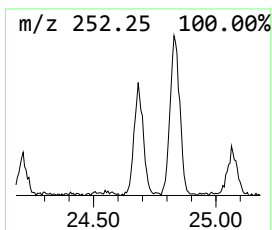
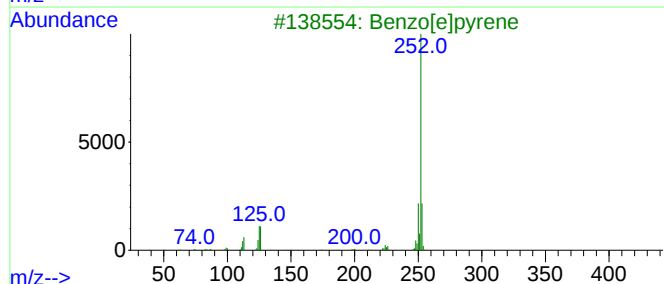
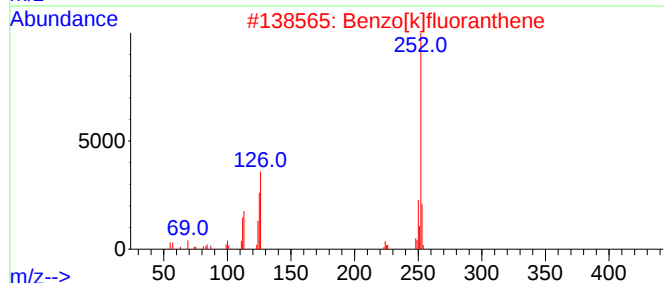
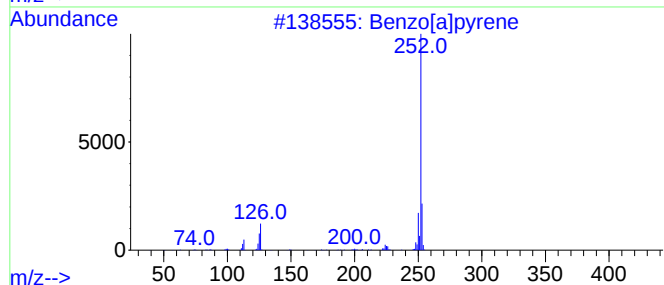
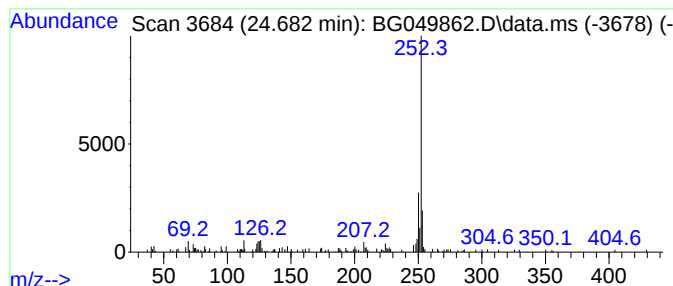
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Benzo[e]pyrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.682	4.74 ng	115285	Perylene-d12	24.994

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[a]pyrene	252	C20H12	000050-32-8	81
2			Benzo[k]fluoranthene	252	C20H12	000207-08-9	81
3			Benzo[e]pyrene	252	C20H12	000192-97-2	81
4			(1-Cyclopentenyl)ferrocene	252	C15H16Fe	012260-67-2	80
5			Benzo[b]fluoranthene	252	C20H12	000205-99-2	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081621\
Data File : BG049862.D
Acq On : 16 Aug 2021 23:13
Operator : CG/JU
Sample : M3404-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP2-1-6FT

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...	3.141	15.9	ng	176593	1	8.028	221396	20.0
2-Pentanone, 4-...	5.109	8.5	ng	94176	1	8.028	221396	20.0
Ethanol, 2-(2-b...	10.607	12.8	ng	194669	2	10.854	305240	20.0
unknown21.340	21.340	2.4	ng	73196	5	21.716	605563	20.0
Benzo[e]pyrene	24.682	4.7	ng	115285	6	24.994	486936	20.0