

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG120722\
 Data File : BG055917.D
 Acq On : 7 Dec 2022 17:00
 Operator : CG/JU
 Sample : N5897-01
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 COMPOSITE

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-BG111622.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055917.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.205	318	326	334	rBV	267374	416502	18.55%	3.278%
2	5.693	402	409	420	rBV	567834	904067	40.27%	7.116%
3	6.304	506	513	521	rVB	17001	27566	1.23%	0.217%
4	7.320	676	686	700	rBV	583058	996162	44.37%	7.841%
5	8.160	823	829	836	rVB	99395	166314	7.41%	1.309%
6	9.335	1021	1029	1041	rBV	354522	619704	27.60%	4.878%
7	10.986	1303	1310	1317	rBV	144644	258397	11.51%	2.034%
8	13.413	1714	1723	1730	rBV	929383	1470357	65.49%	11.574%
9	14.206	1854	1858	1862	rBV3	12845	23373	1.04%	0.184%
10	14.523	1907	1912	1918	rBV9	10700	24755	1.10%	0.195%
11	14.794	1952	1958	1965	rVB	247678	394219	17.56%	3.103%
12	16.139	2181	2187	2193	rVB	159262	239604	10.67%	1.886%
13	16.280	2205	2211	2230	rVB	798789	1259561	56.10%	9.915%
14	16.486	2239	2246	2254	rVB7	14828	39147	1.74%	0.308%
15	16.697	2278	2282	2288	rBV4	14131	22602	1.01%	0.178%
16	17.532	2418	2424	2429	rBV	323245	525989	23.43%	4.140%
17	17.579	2429	2432	2437	rVB	105665	142019	6.33%	1.118%
18	18.401	2567	2572	2577	rBV2	63910	113624	5.06%	0.894%
19	18.454	2578	2581	2587	rVB2	29144	46588	2.08%	0.367%
20	18.601	2601	2606	2617	rVB5	31677	93813	4.18%	0.738%
21	19.306	2722	2726	2732	rBV3	25778	56434	2.51%	0.444%
22	19.576	2767	2772	2776	rBV	178062	248865	11.08%	1.959%
23	19.617	2776	2779	2783	rVB2	42213	53415	2.38%	0.420%
24	19.676	2784	2789	2792	rBV6	14145	25637	1.14%	0.202%
25	19.905	2824	2828	2830	rBV2	34373	54223	2.42%	0.427%
26	19.941	2830	2834	2841	rVV	158352	227659	10.14%	1.792%
27	20.005	2841	2845	2850	rVB2	17266	25384	1.13%	0.200%
28	20.123	2859	2865	2871	rVB	1763785	2245125	100.00%	17.672%
29	20.264	2884	2889	2896	rVB2	19116	41123	1.83%	0.324%
30	20.334	2898	2901	2906	rVV	38335	50734	2.26%	0.399%
31	20.405	2909	2913	2914	rVV3	27007	41234	1.84%	0.325%
32	20.422	2914	2916	2922	rVB2	37137	46065	2.05%	0.363%
33	20.522	2930	2933	2937	rVB2	23446	27210	1.21%	0.214%
34	21.415	3081	3085	3094	rBV3	68408	151259	6.74%	1.191%
35	21.815	3145	3153	3158	rBV3	346299	696560	31.03%	5.483%
36	21.862	3158	3161	3168	rVB	75126	115374	5.14%	0.908%

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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-BG111622.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	24.089	3535	3540	3549	rBV	40146	146723	6.54%	1.155%
38	24.999	3689	3695	3704	rVB	52426	135913	6.05%	1.070%
39	25.158	3714	3722	3733	rVB2	192303	530919	23.65%	4.179%

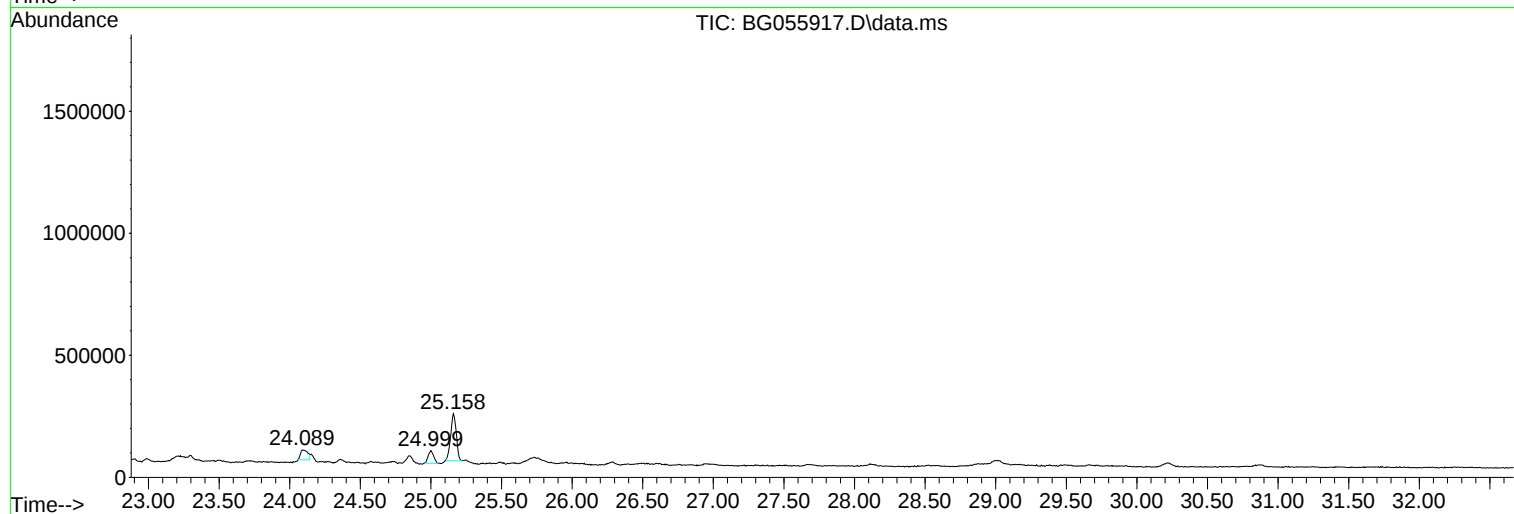
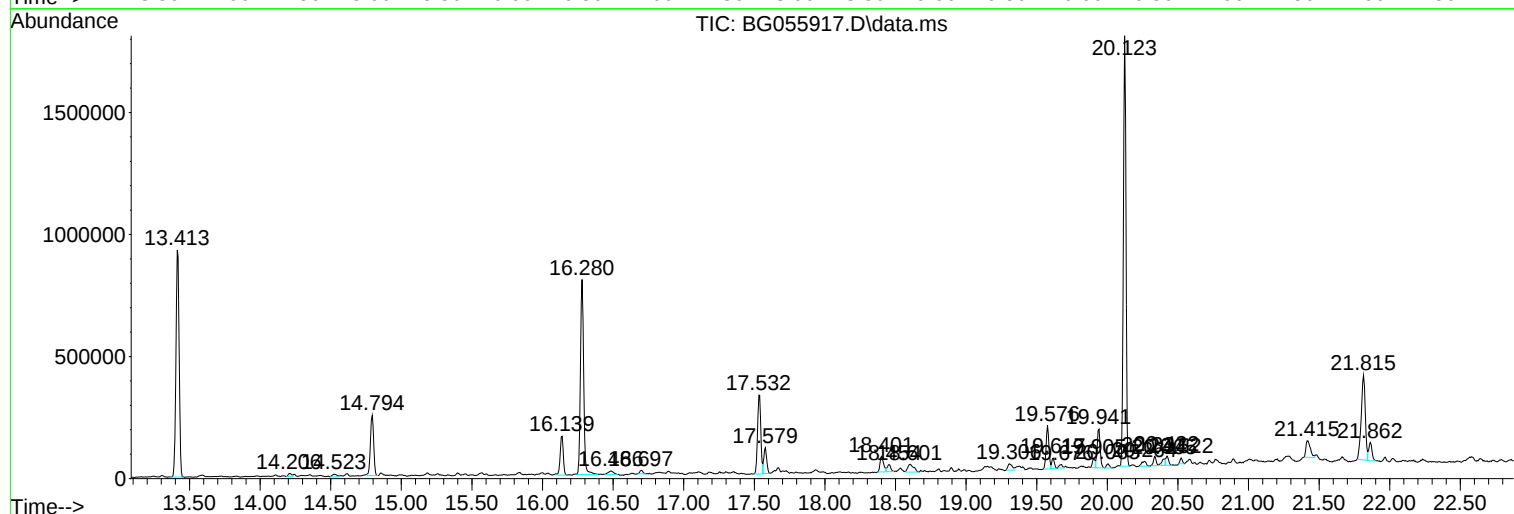
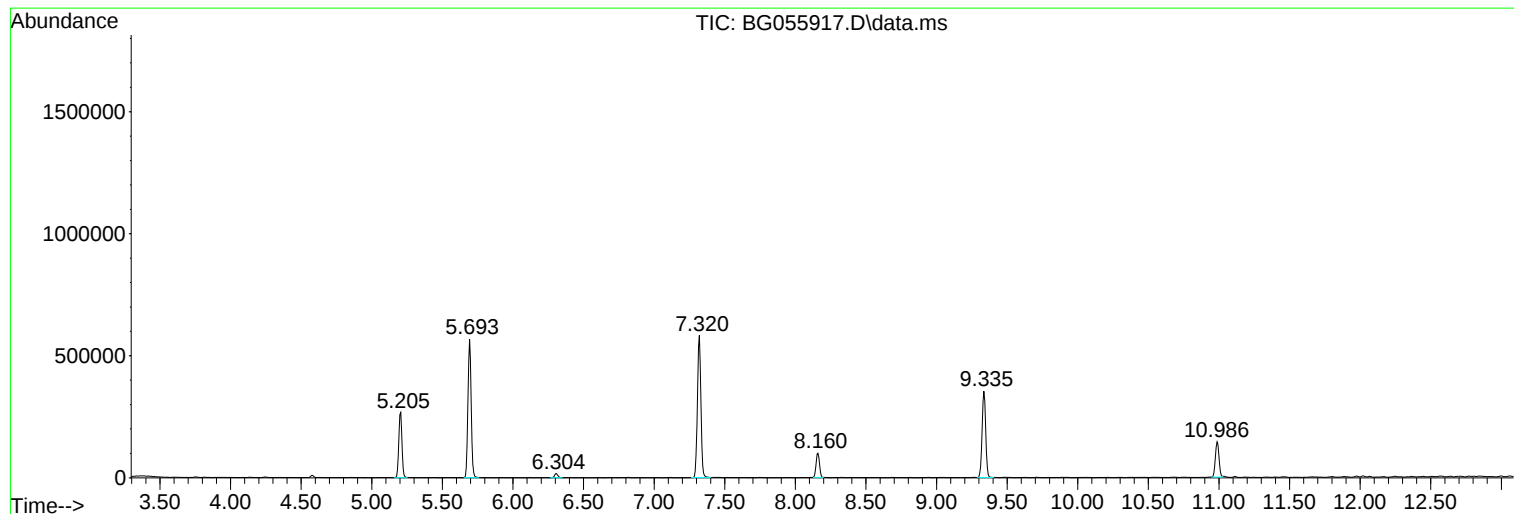
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Operator : CG/JU
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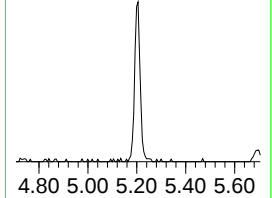
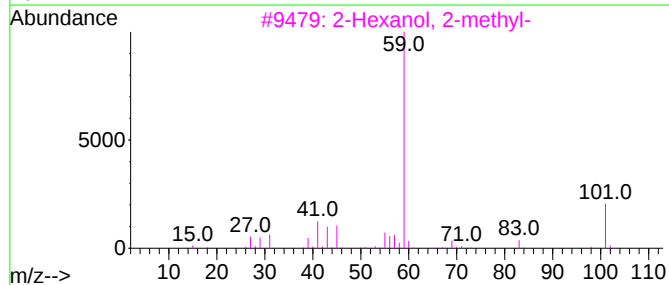
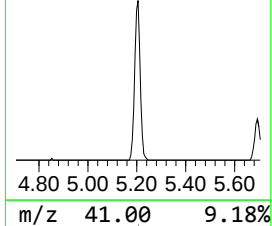
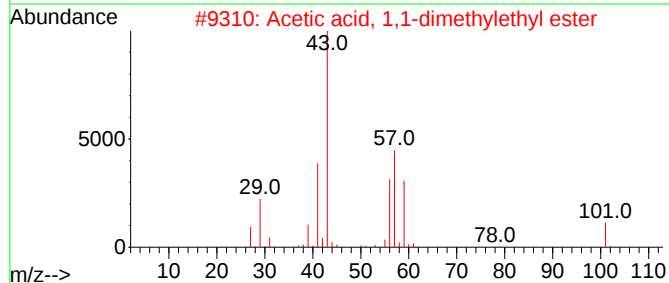
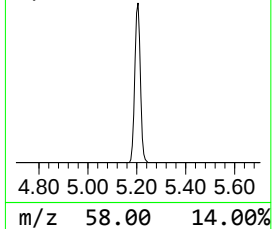
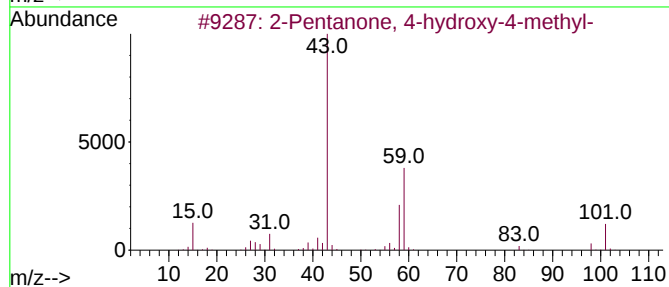
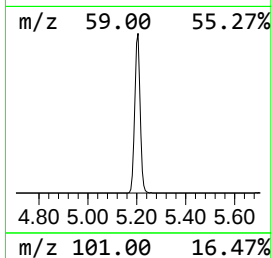
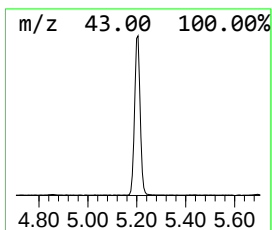
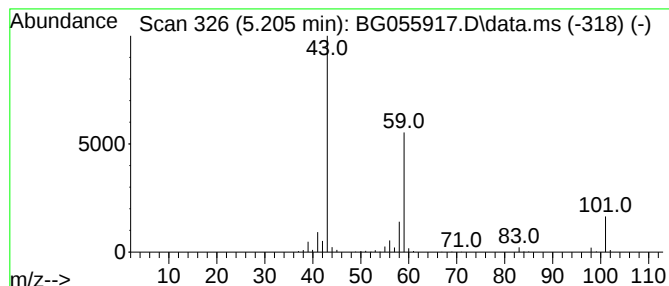
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.205	50.09 ng	416502	1,4-Dichlorobenzene-d4	8.160

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12



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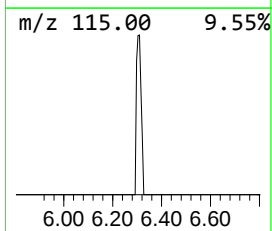
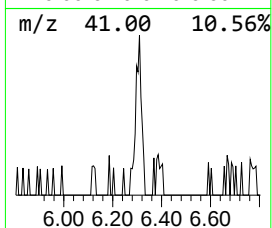
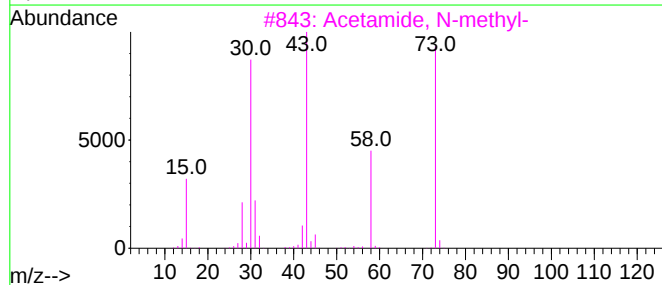
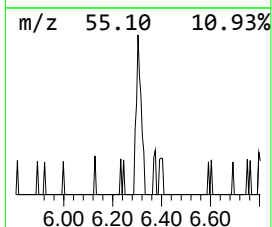
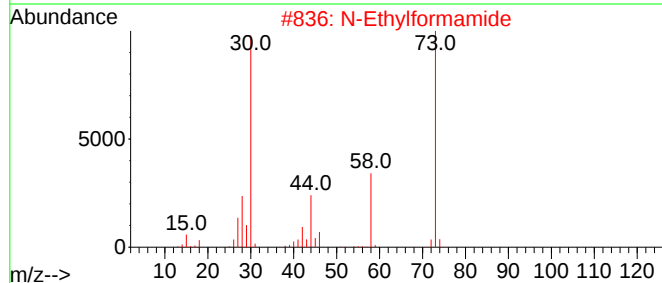
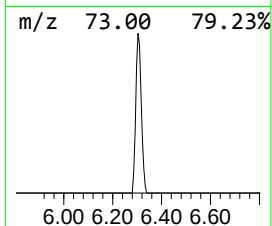
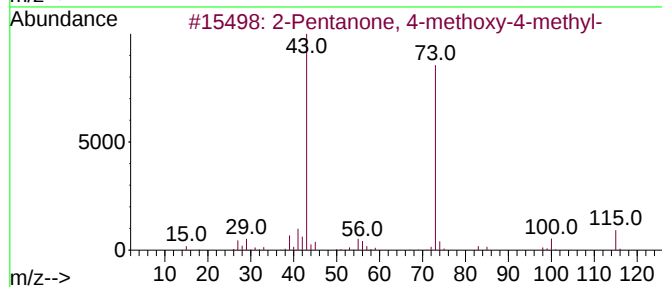
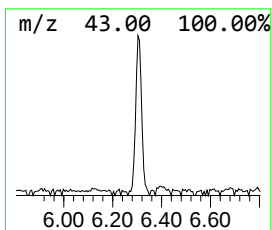
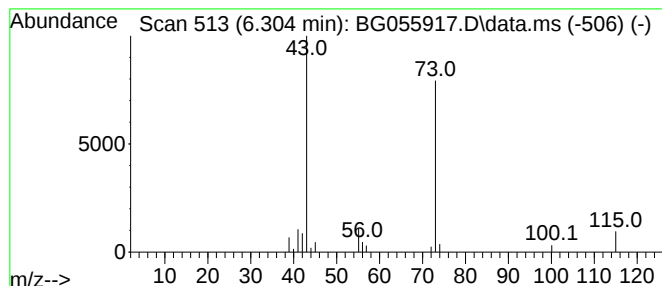
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-methoxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.304	3.31 ng	27566	1,4-Dichlorobenzene-d4	8.160

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	78
2			N-Ethylformamide	73	C3H7NO	000627-45-2	32
3			Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9
4			1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	9
5			Isobutyl acetate	116	C6H12O2	000110-19-0	9



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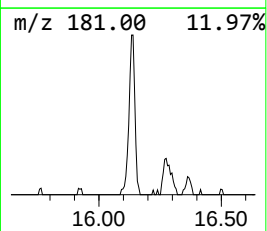
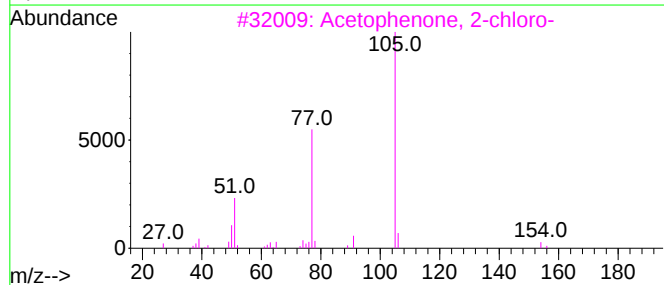
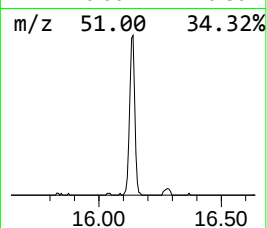
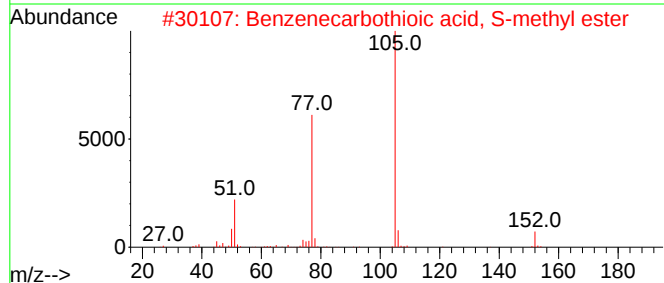
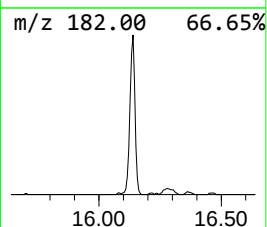
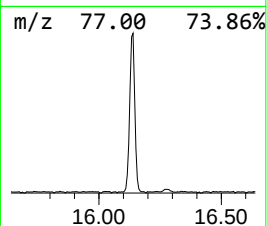
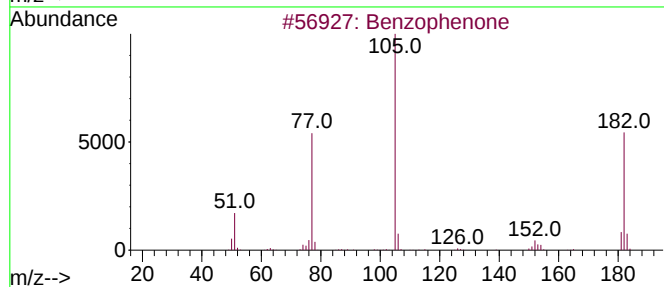
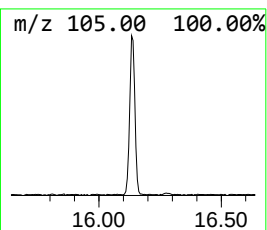
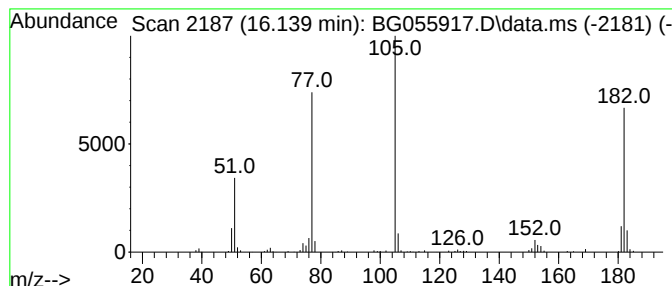
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.139	12.16 ng	239604	Acenaphthene-d10	14.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	58
3			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	52
4			Glyoxylohydroximoyl chloride, 2-...	183	C8H6ClNO2	004937-87-5	52
5			Disulfide, dibenzoyl	274	C14H10O2S2	000644-32-6	50



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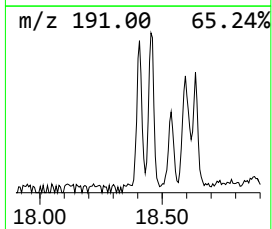
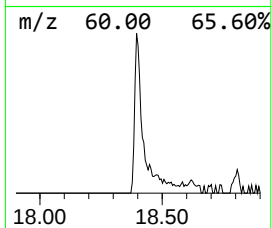
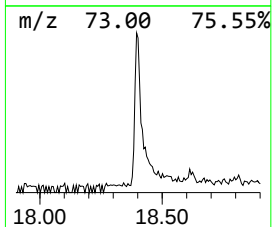
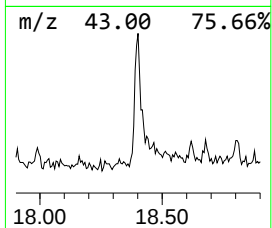
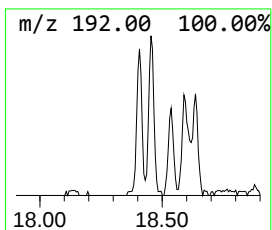
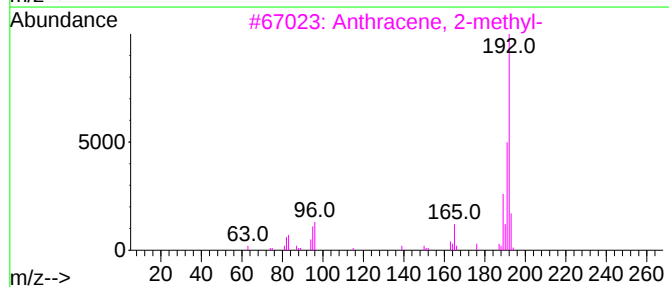
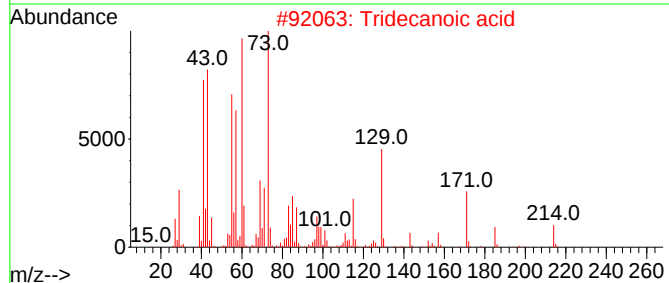
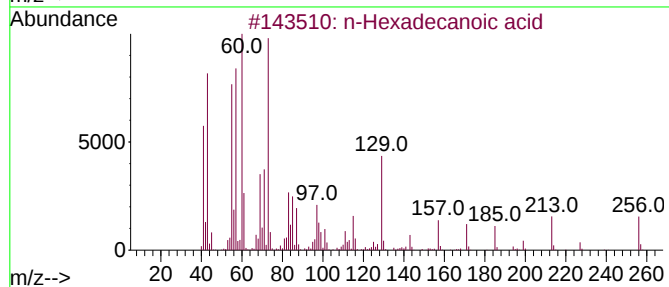
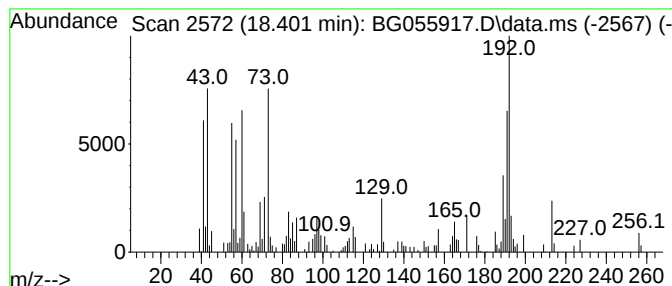
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.401	4.32 ng	113624	Phenanthrene-d10	17.532

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2			Tridecanoic acid	214	C13H26O2	000638-53-9	60
3			Anthracene, 2-methyl-	192	C15H12	000613-12-7	55
4			Anthracene, 1-methyl-	192	C15H12	000610-48-0	46
5			Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	46



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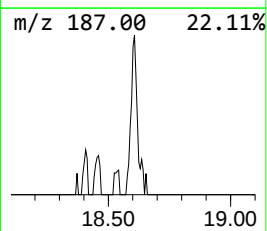
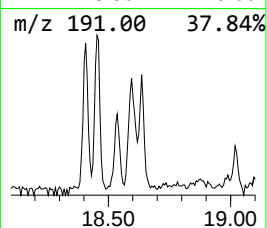
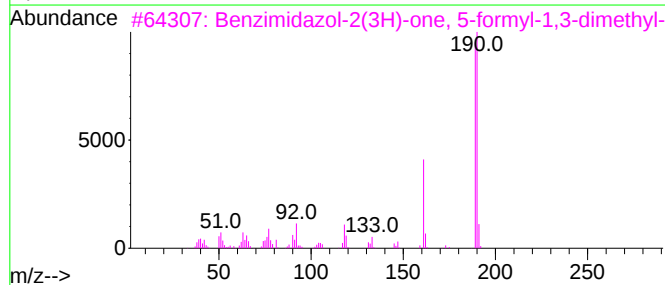
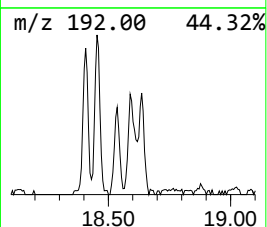
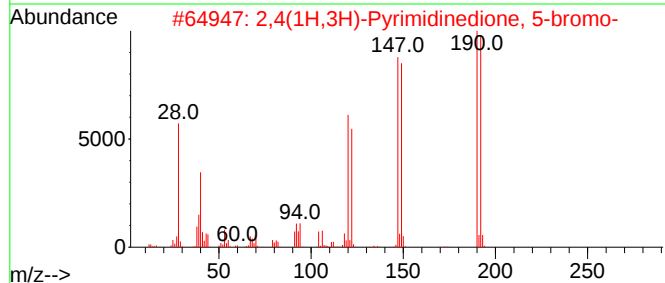
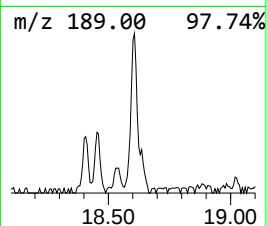
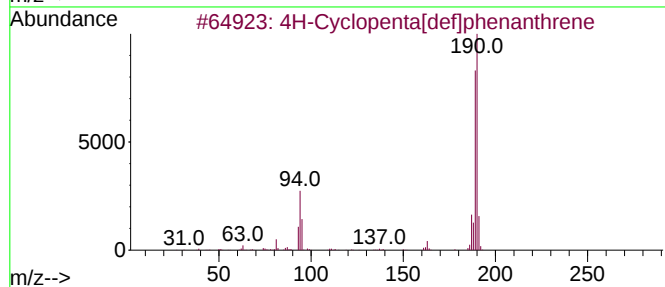
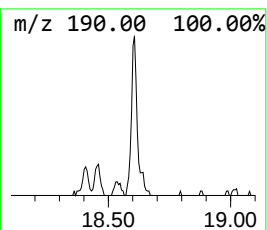
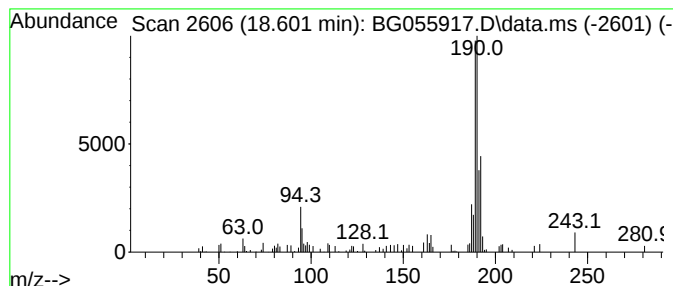
Instrument :
BNA_G
ClientSampleId :
COMPOSITE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 4H-Cyclopenta[def]phenanthrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.601	3.57 ng	93813	Phenanthrene-d10	17.532	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	68
2	2,4(1H,3H)-Pyrimidinedione, 5-br...	190	C4H3BrN2O2	000051-20-7	38
3	Benzimidazol-2(3H)-one, 5-formyl...	190	C10H10N2O2	055241-49-1	37
4	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	35
5	Carbonic acid, 2-formyl-4,6-dich...	276	C11H10Cl2O4	1000331-39-3	32



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG120722\
Data File : BG055917.D
Acq On : 7 Dec 2022 17:00
Operator : CG/JU
Sample : N5897-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COMPOSITE

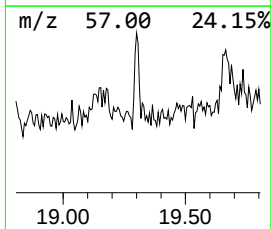
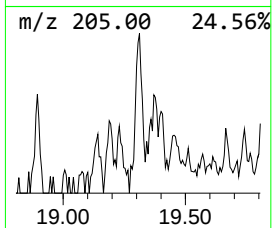
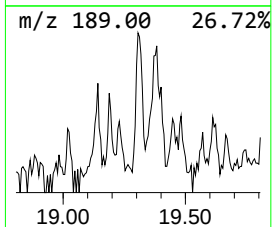
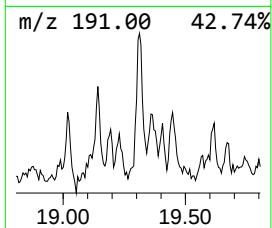
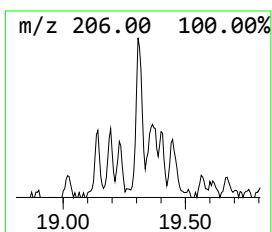
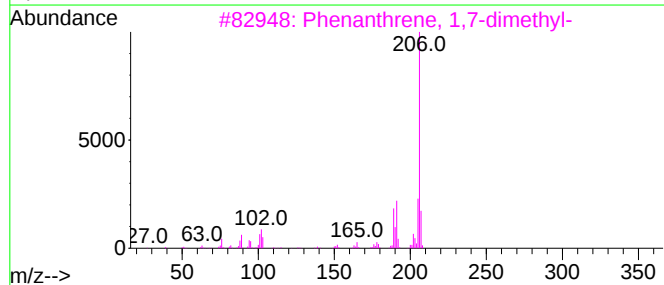
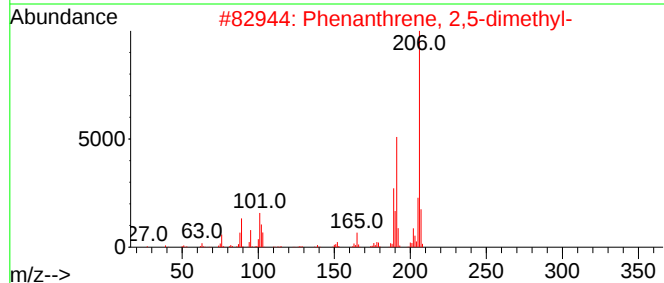
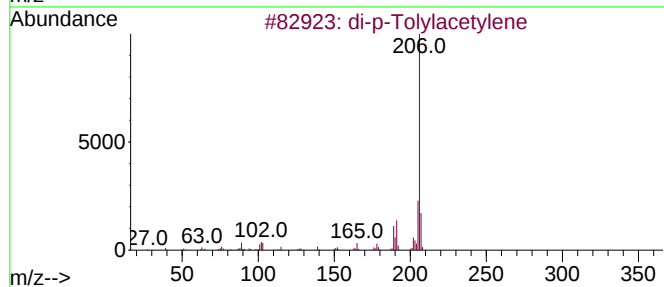
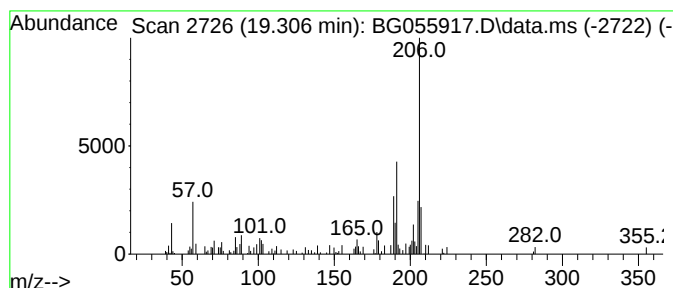
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 di-p-Tolylacetylene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.306	2.15 ng	56434	Phenanthrene-d10	17.532

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			di-p-Tolylacetylene	206	C16H14	002789-88-0	93
2			Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	91
3			Phenanthrene, 1,7-dimethyl-	206	C16H14	000483-87-4	91
4			3,4-Dimethylphenanthrene	206	C16H14	1000452-24-5	80
5			Phenanthrene, 3,6-dimethyl-	206	C16H14	001576-67-6	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG120722\
Data File : BG055917.D
Acq On : 7 Dec 2022 17:00
Operator : CG/JU
Sample : N5897-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COMPOSITE

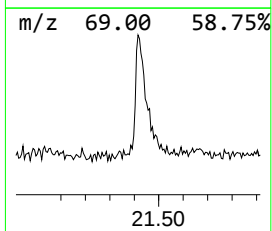
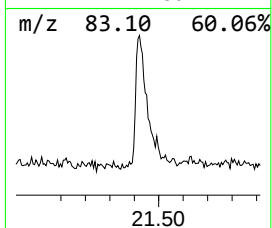
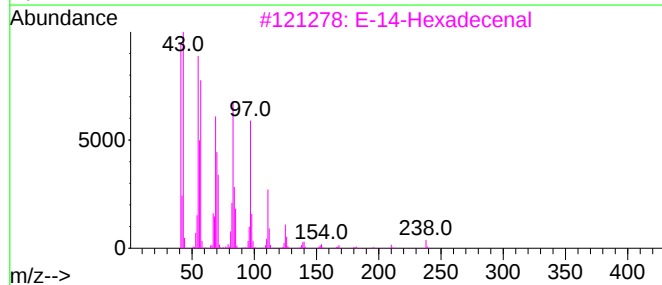
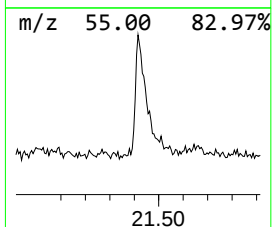
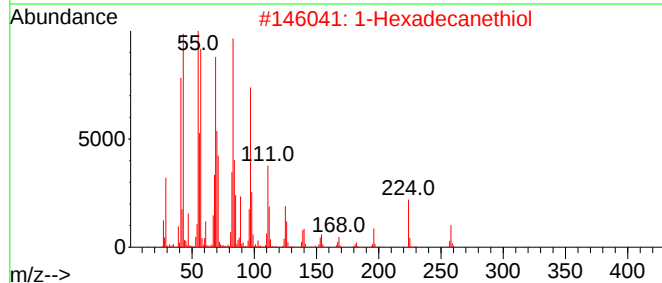
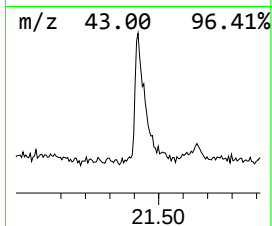
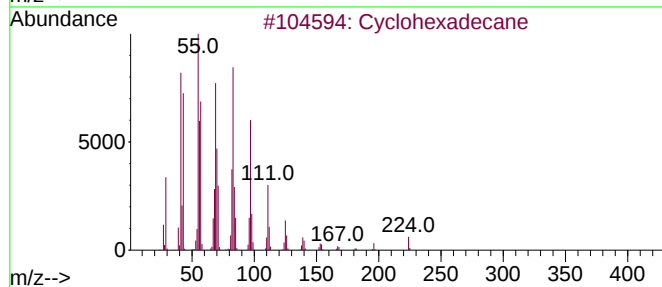
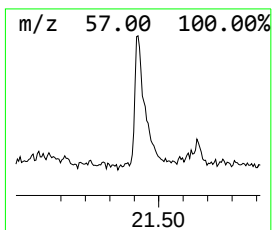
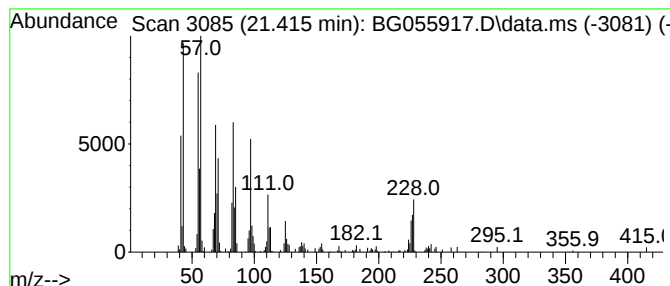
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Cyclohexadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.415	4.34 ng	151259	Chrysene-d12	21.815

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexadecane	224	C16H32	000295-65-8	98
2			1-Hexadecanethiol	258	C16H34S	002917-26-2	90
3			E-14-Hexadecenal	238	C16H30O	330207-53-9	89
4			Cyclotetracosane	336	C24H48	000297-03-0	87
5			Nonacos-1-ene	406	C29H58	018835-35-3	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG120722\
Data File : BG055917.D
Acq On : 7 Dec 2022 17:00
Operator : CG/JU
Sample : N5897-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COMPOSITE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.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-...	5.205	50.1	ng	416502	1	8.160	166314	20.0
2-Pentanone, 4-...	6.304	3.3	ng	27566	1	8.160	166314	20.0
Benzophenone	16.139	12.2	ng	239604	3	14.794	394219	20.0
n-Hexadecanoic ...	18.401	4.3	ng	113624	4	17.532	525989	20.0
4H-Cyclopenta[d]...	18.601	3.6	ng	93813	4	17.532	525989	20.0
di-p-Tolylacety...	19.306	2.1	ng	56434	4	17.532	525989	20.0
Cyclohexadecane	21.415	4.3	ng	151259	5	21.815	696560	20.0