

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121922\
 Data File : BG056016.D
 Acq On : 19 Dec 2022 16:46
 Operator : CG/JU
 Sample : N6037-23
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 RB-28-(2.5-4.5)

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-BG121322.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG056016.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.399	14	19	26	rBV2	26279	38877	5.21%	1.020%
2	5.415	356	362	368	rBB	14860	22877	3.07%	0.600%
3	5.885	436	442	449	rBB	122406	187393	25.12%	4.919%
4	7.495	709	716	723	rBB	118756	205868	27.60%	5.404%
5	8.364	859	864	871	rBB	33231	55057	7.38%	1.445%
6	9.539	1057	1064	1071	rBB	76477	131877	17.68%	3.461%
7	11.202	1340	1347	1354	rBB	44439	76576	10.27%	2.010%
8	13.605	1749	1756	1762	rBB	250437	382281	51.25%	10.034%
9	14.974	1983	1989	1995	rBB	84378	127112	17.04%	3.336%
10	16.314	2212	2217	2222	rBB2	14861	21975	2.95%	0.577%
11	16.449	2234	2240	2247	rBV	327652	492570	66.03%	12.929%
12	17.712	2448	2455	2459	rBV	122053	184567	24.74%	4.844%
13	17.753	2459	2462	2469	rVB	20893	28144	3.77%	0.739%
14	18.558	2594	2599	2606	rBV4	35335	54438	7.30%	1.429%
15	18.629	2606	2611	2616	rVB	7162	11228	1.51%	0.295%
16	18.764	2629	2634	2638	rBV2	6202	12760	1.71%	0.335%
17	18.805	2638	2641	2646	rVB2	5012	7607	1.02%	0.200%
18	19.105	2688	2692	2697	rVB3	6044	8780	1.18%	0.230%
19	19.475	2749	2755	2759	rBV4	5172	7889	1.06%	0.207%
20	19.739	2795	2800	2805	rVB	46825	66387	8.90%	1.742%
21	19.810	2806	2812	2820	rBV7	9502	15502	2.08%	0.407%
22	20.098	2849	2861	2867	rBV	54565	85380	11.45%	2.241%
23	20.286	2887	2893	2898	rBV	592258	745972	100.00%	19.580%
24	20.427	2910	2917	2922	rVB5	4751	10121	1.36%	0.266%
25	20.738	2965	2970	2975	rBV3	6504	10354	1.39%	0.272%
26	20.885	2991	2995	2999	rBV	6330	10611	1.42%	0.279%
27	20.932	2999	3003	3008	rVV3	6416	9435	1.26%	0.248%
28	21.367	3073	3077	3083	rBV2	6714	12088	1.62%	0.317%
29	21.608	3113	3118	3124	rVB2	25819	41158	5.52%	1.080%
30	21.719	3133	3137	3142	rBV3	5255	8069	1.08%	0.212%
31	22.019	3179	3188	3193	rBV3	133935	278173	37.29%	7.301%
32	22.066	3193	3196	3203	rVB	24512	40565	5.44%	1.065%
33	22.806	3318	3322	3327	rVB4	4789	8446	1.13%	0.222%
34	22.871	3329	3333	3342	rVB7	6279	12814	1.72%	0.336%
35	23.823	3490	3495	3501	rVB4	12123	25084	3.36%	0.658%
36	24.393	3583	3592	3600	rBV2	16927	59881	8.03%	1.572%

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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-BG121322.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	25.174	3720	3725	3738	rVB2	12371	38584	5.17%	1.013%
38	25.333	3746	3752	3753	rBV5	13609	20058	2.69%	0.526%
39	25.509	3771	3782	3792	rBV2	79995	237541	31.84%	6.235%
40	29.522	4458	4465	4471	rBV4	5151	15783	2.12%	0.414%

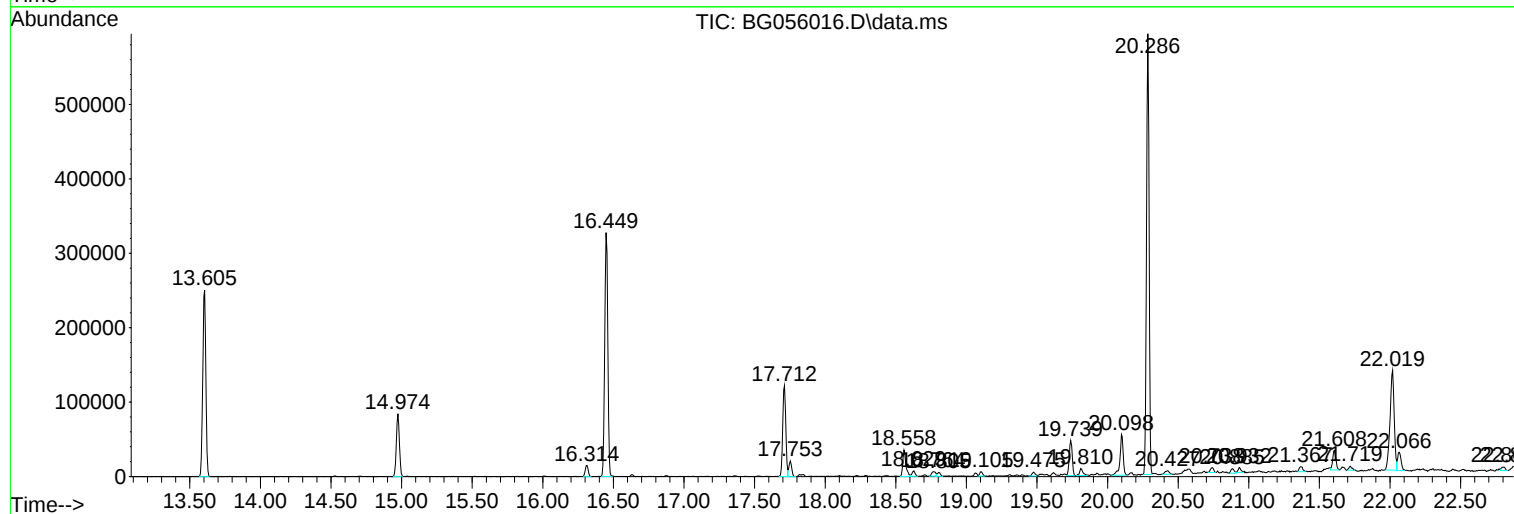
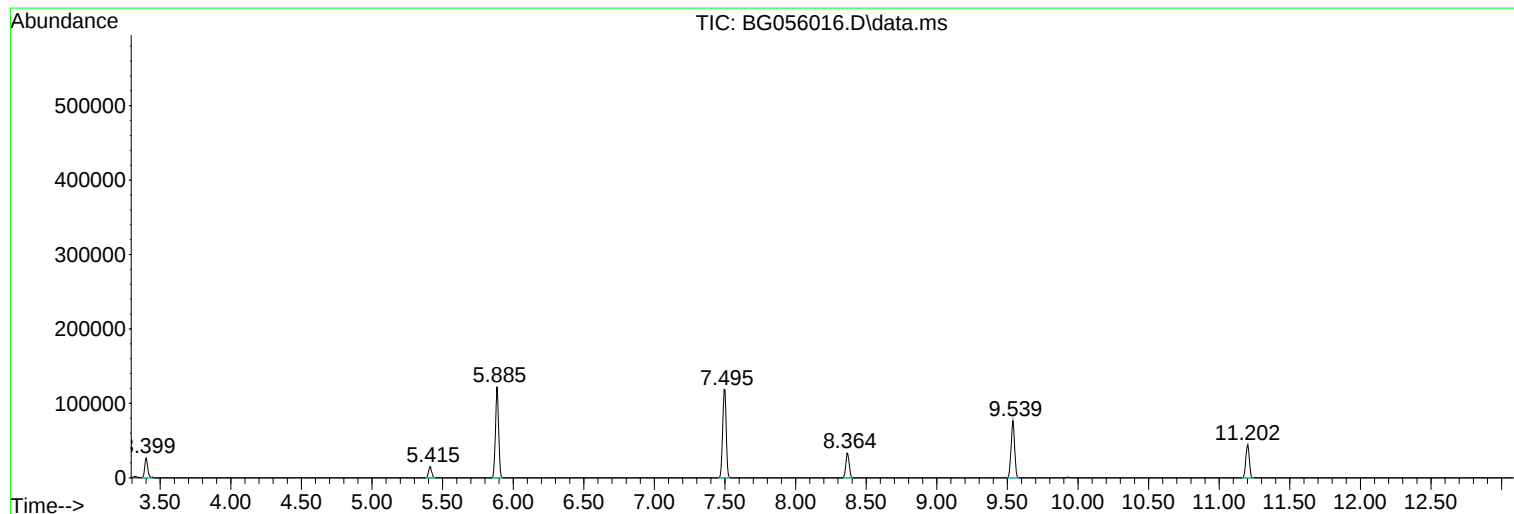
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RB-28-(2.5-4.5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.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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BNA_G
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RB-28-(2.5-4.5)

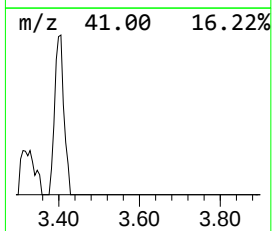
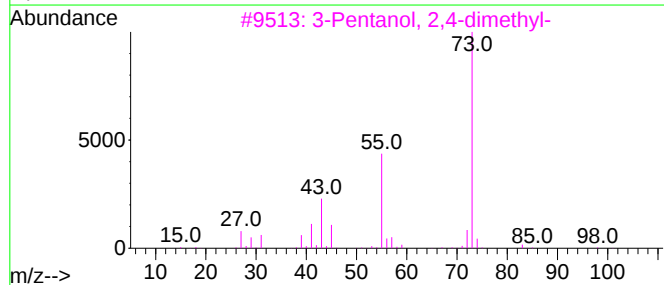
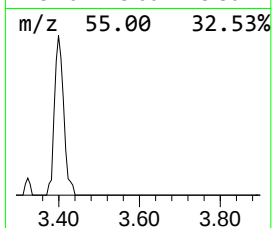
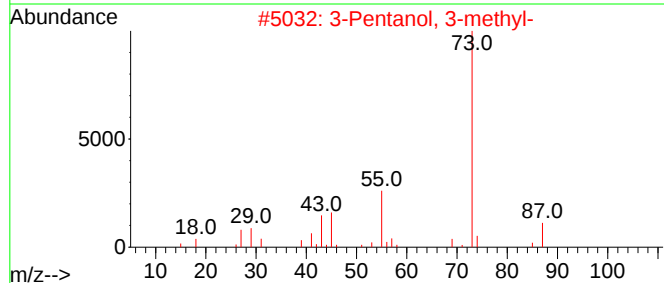
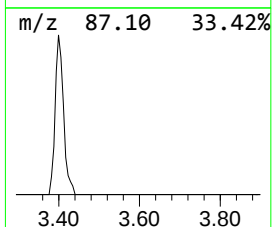
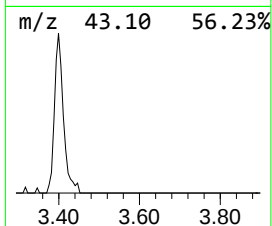
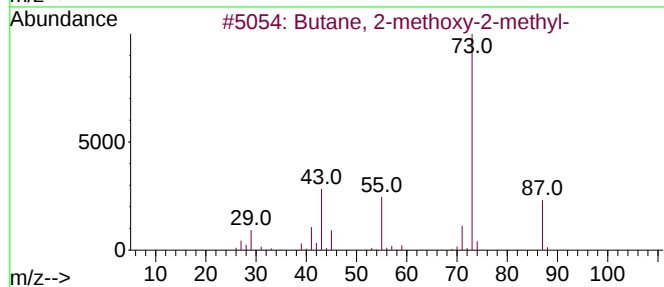
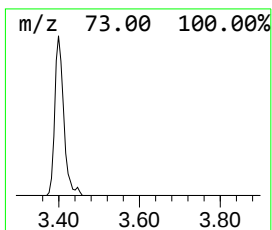
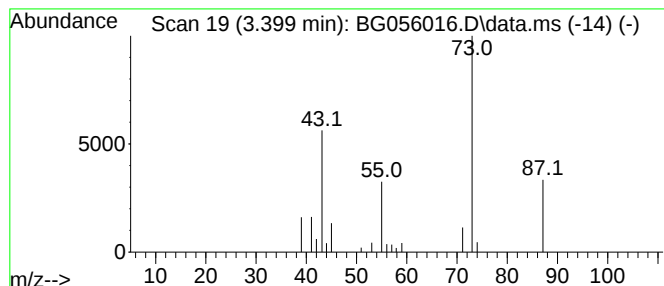
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
3.399	14.12 ng	38877	1,4-Dichlorobenzene-d4	8.370

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	36
3			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	25
4			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	25
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17



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ClientSampleId :
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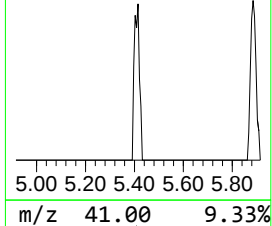
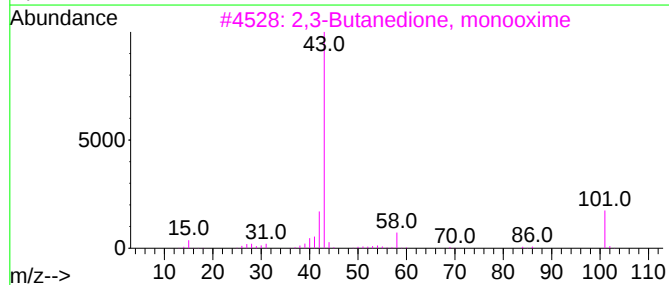
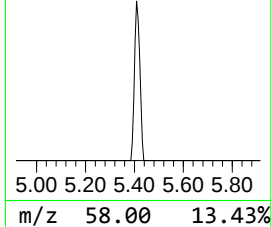
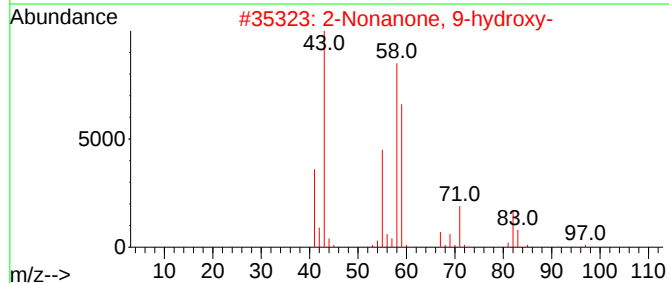
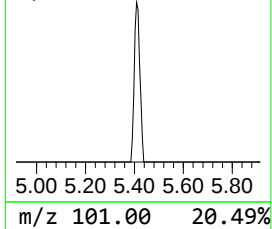
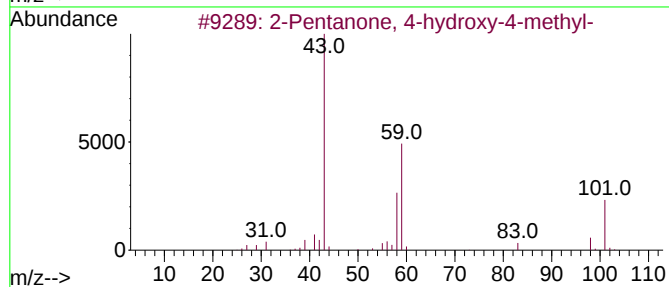
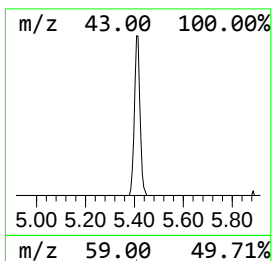
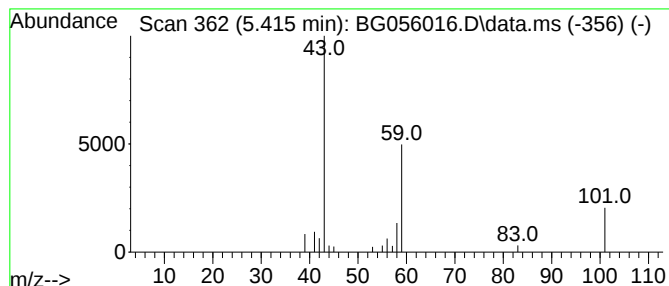
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.415	8.31 ng	22877	1,4-Dichlorobenzene-d4	8.370

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	78
2		2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	33
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9
5		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9



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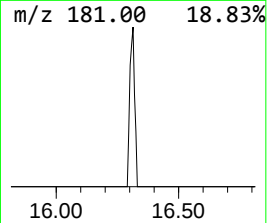
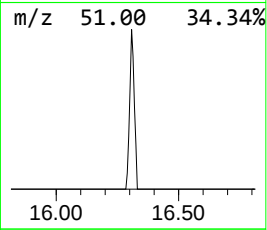
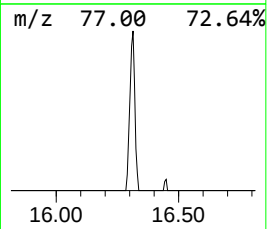
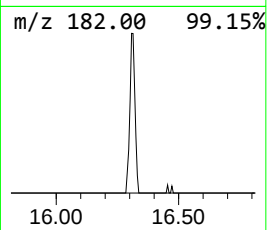
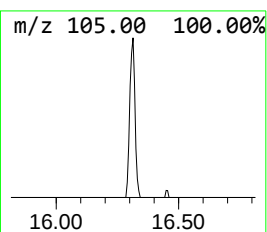
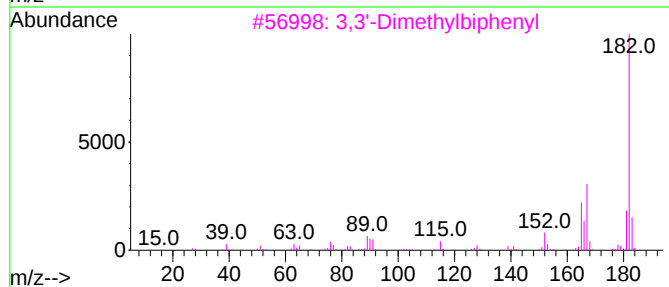
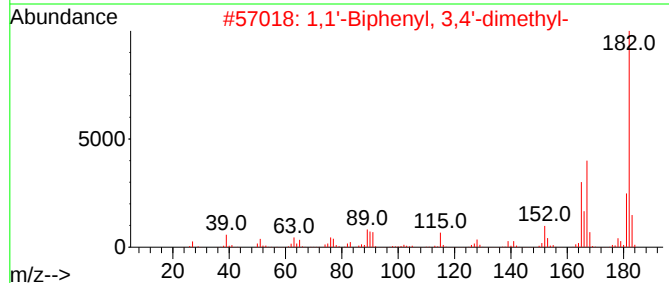
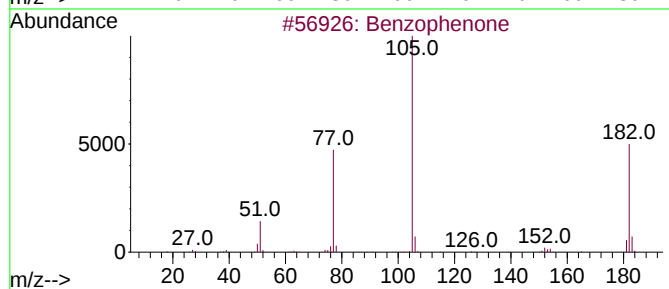
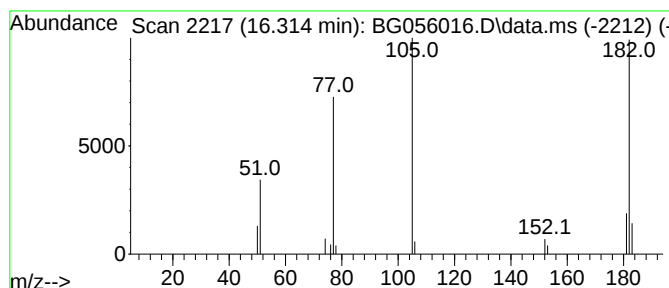
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.314	3.46 ng	21975	Acenaphthene-d10	14.974

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	91
2			1,1'-Biphenyl, 3,4'-dimethyl-	182	C14H14	007383-90-6	46
3			3,3'-Dimethylbiphenyl	182	C14H14	000612-75-9	43
4			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	38
5			Methanone, phenyl-2-pyridinyl-	183	C12H9NO	000091-02-1	38



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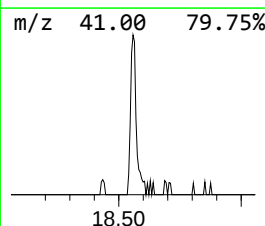
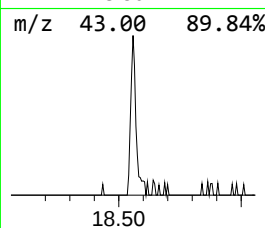
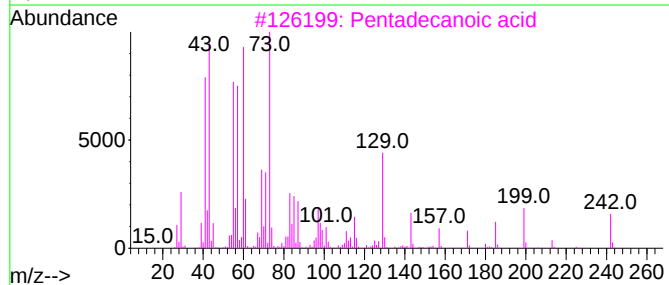
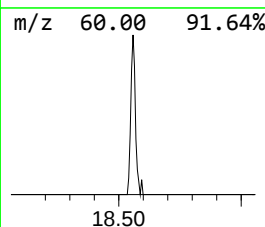
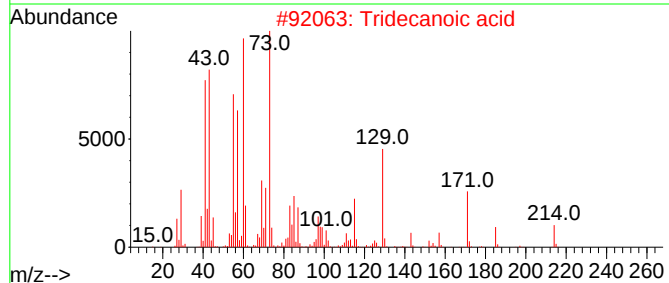
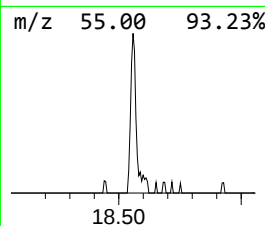
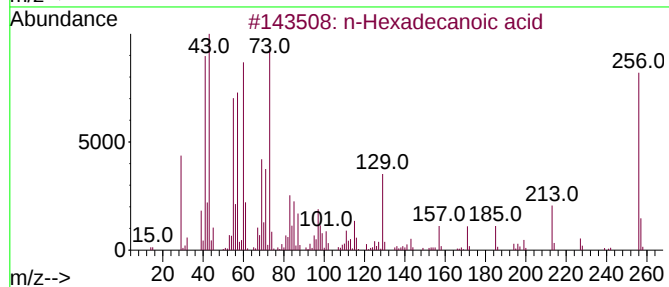
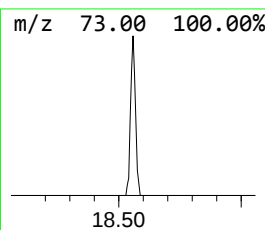
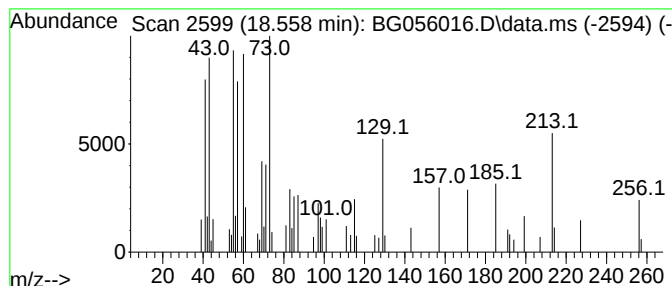
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.558	5.90 ng	54438	Phenanthrene-d10	17.712

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2			Tridecanoic acid	214	C13H26O2	000638-53-9	95
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	60
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	58
5			Dodecanoic acid	200	C12H24O2	000143-07-7	46



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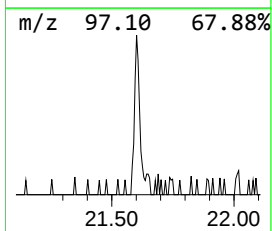
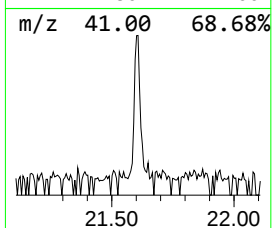
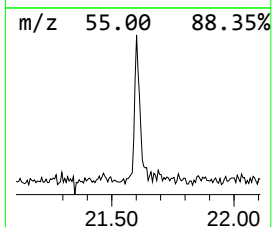
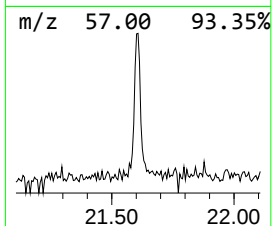
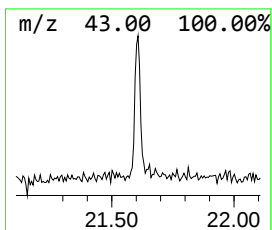
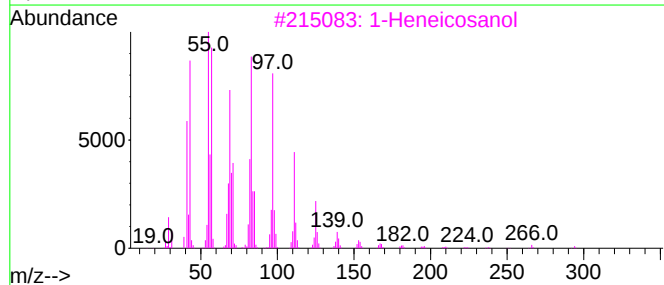
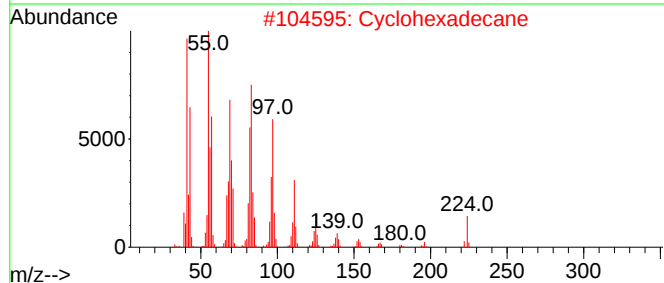
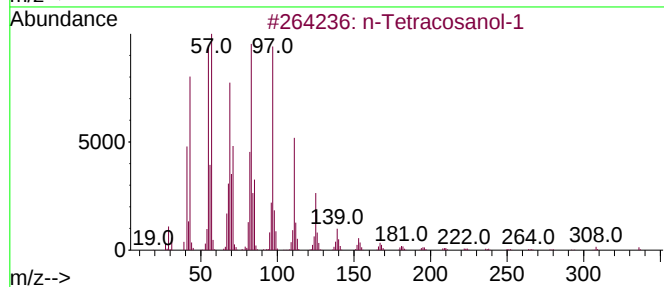
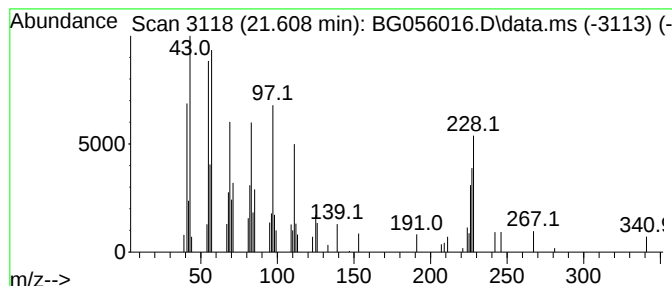
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 n-Tetracosanol-1 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.608	2.96 ng	41158	Chrysene-d12	22.019

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Tetracosanol-1	354	C24H50O	000506-51-4	84
2			Cyclohexadecane	224	C16H32	000295-65-8	70
3			1-Heneicosanol	312	C21H44O	015594-90-8	50
4			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	50
5			Octacosanol	410	C28H58O	000557-61-9	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121922\
Data File : BG056016.D
Acq On : 19 Dec 2022 16:46
Operator : CG/JU
Sample : N6037-23
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RB-28-(2.5-4.5)

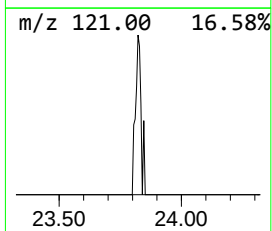
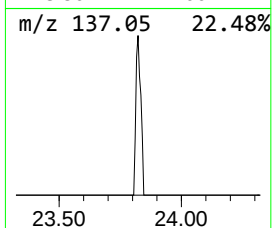
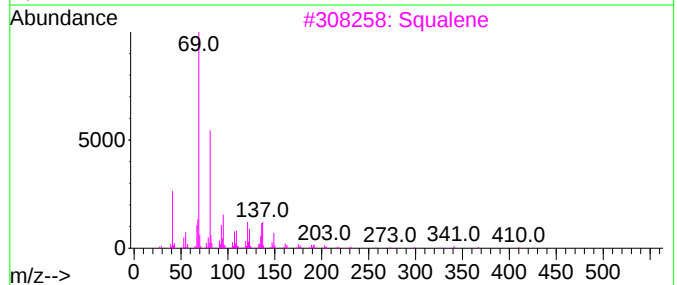
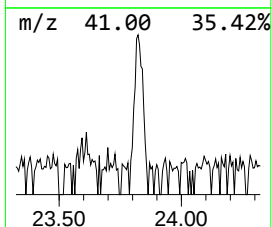
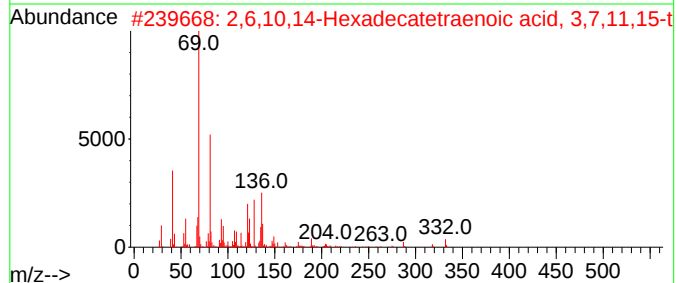
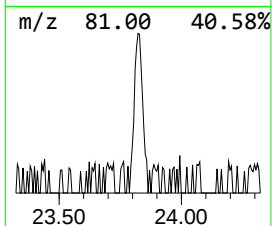
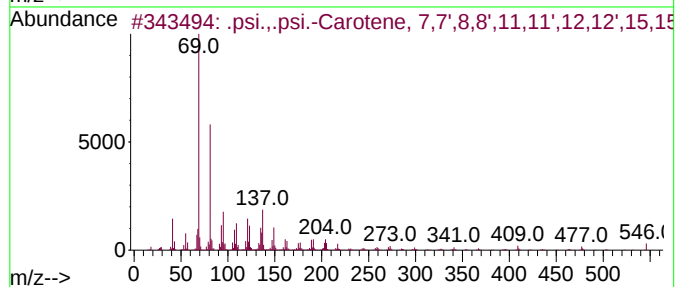
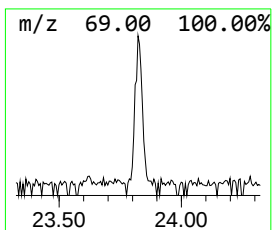
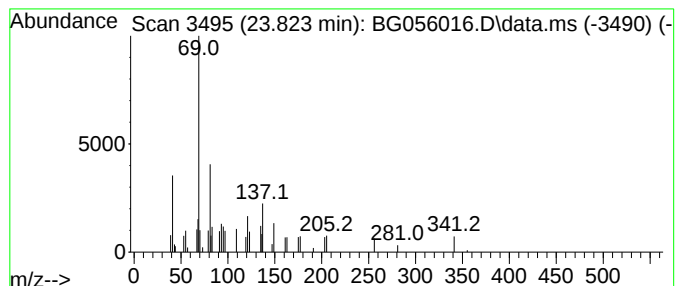
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 .psi.,.psi.-Carotene, 7,7',... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.823	2.11 ng	25084	Perylene-d12	25.509

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	72		
2	2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	64		
3	Squalene	410	C30H50	000111-02-4	59		
4	5,9,13,17-Tetramethyl 4,8,12,16-...	332	C22H36O2	1000432-37-9	59		
5	(2E,6E)-3,7,11-Trimethyldodeca-2...	404	C27H48O2	078368-58-8	59		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121922\
Data File : BG056016.D
Acq On : 19 Dec 2022 16:46
Operator : CG/JU
Sample : N6037-23
Misc :
ALS Vial : 9 Sample Multiplier: 1

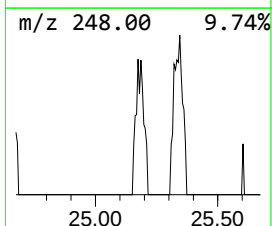
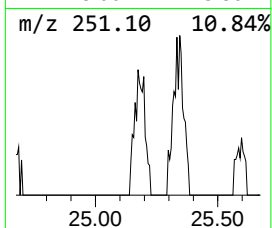
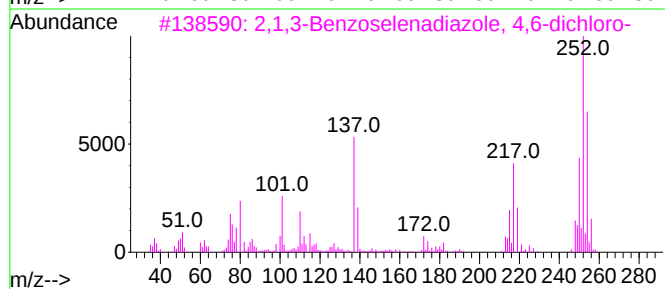
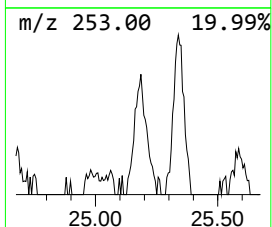
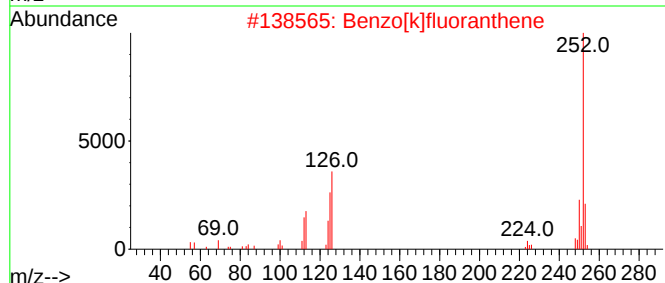
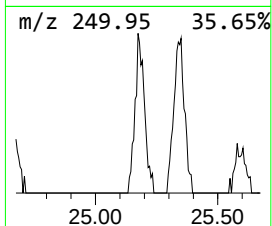
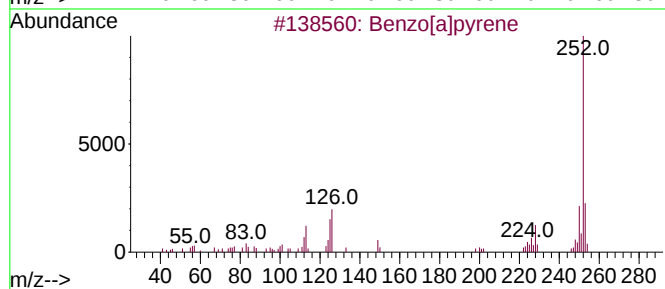
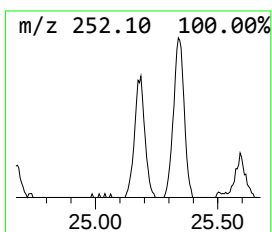
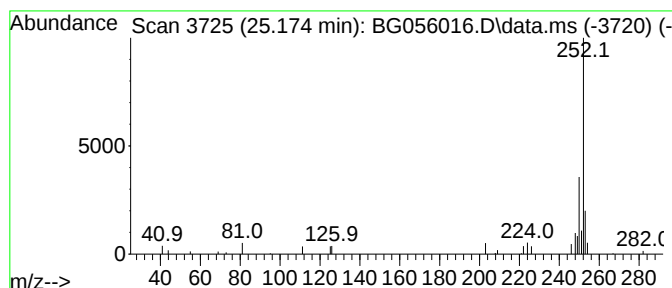
Instrument :
BNA_G
ClientSampleId :
RB-28-(2.5-4.5)

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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 7 2,1,3-Benzoselenadiazole, 4... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
25.174	3.25 ng	38584	Perylene-d12	25.509	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[a]pyrene	252	C20H12	000050-32-8	72
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	72
3	2,1,3-Benzoselenadiazole, 4,6-di...	252	C6H2Cl2N2Se	090030-99-2	64
4	Benzo[e]pyrene	252	C20H12	000192-97-2	59
5	Perylene	252	C20H12	000198-55-0	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121922\
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Sample : N6037-23
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RB-28-(2.5-4.5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.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
Butane, 2-metho...	3.399	14.1	ng	38877	1	8.370	55057	20.0
2-Pentanone, 4-...	5.415	8.3	ng	22877	1	8.370	55057	20.0
Benzophenone	16.314	3.5	ng	21975	3	14.974	127112	20.0
n-Hexadecanoic ...	18.558	5.9	ng	54438	4	17.712	184567	20.0
n-Tetracosanol-1	21.608	3.0	ng	41158	5	22.019	278173	20.0
.psi.,.psi.-Car...	23.823	2.1	ng	25084	6	25.509	237541	20.0
2,1,3-Benzosele...	25.174	3.3	ng	38584	6	25.509	237541	20.0