

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112522\
 Data File : BG055779.D
 Acq On : 25 Nov 2022 13:36
 Operator : CG/JU
 Sample : N5741-02
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 MW-15

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: BG055779.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.836	88	93	99	rBV	19921	29164	1.25%	0.284%
2	5.288	332	340	347	rBV	51586	80932	3.46%	0.789%
3	5.764	415	421	433	rBV	256633	431828	18.45%	4.210%
4	7.379	689	696	706	rBV	163813	293119	12.52%	2.858%
5	8.237	835	842	848	rBV	119604	200541	8.57%	1.955%
6	8.449	872	878	884	rVB2	29335	47597	2.03%	0.464%
7	9.406	1033	1041	1052	rBV	341431	597426	25.53%	5.824%
8	11.063	1316	1323	1335	rVB	170271	302036	12.90%	2.945%
9	13.484	1728	1735	1744	rVB	925471	1473166	62.94%	14.362%
10	14.859	1961	1969	1978	rBV	314963	474125	20.26%	4.622%
11	16.204	2191	2198	2205	rVB	40818	64935	2.77%	0.633%
12	16.345	2215	2222	2234	rBV	893988	1417160	60.55%	13.816%
13	17.603	2429	2436	2445	rBV	412401	621930	26.57%	6.063%
14	18.461	2578	2582	2606	rBV4	69830	227590	9.72%	2.219%
15	19.718	2792	2796	2818	rVB2	91298	243630	10.41%	2.375%
16	20.188	2870	2876	2882	rVB	1813462	2340529	100.00%	22.818%
17	21.898	3161	3167	3175	rVB	406454	677226	28.93%	6.602%
18	25.294	3737	3745	3758	rVB2	242396	734282	31.37%	7.159%

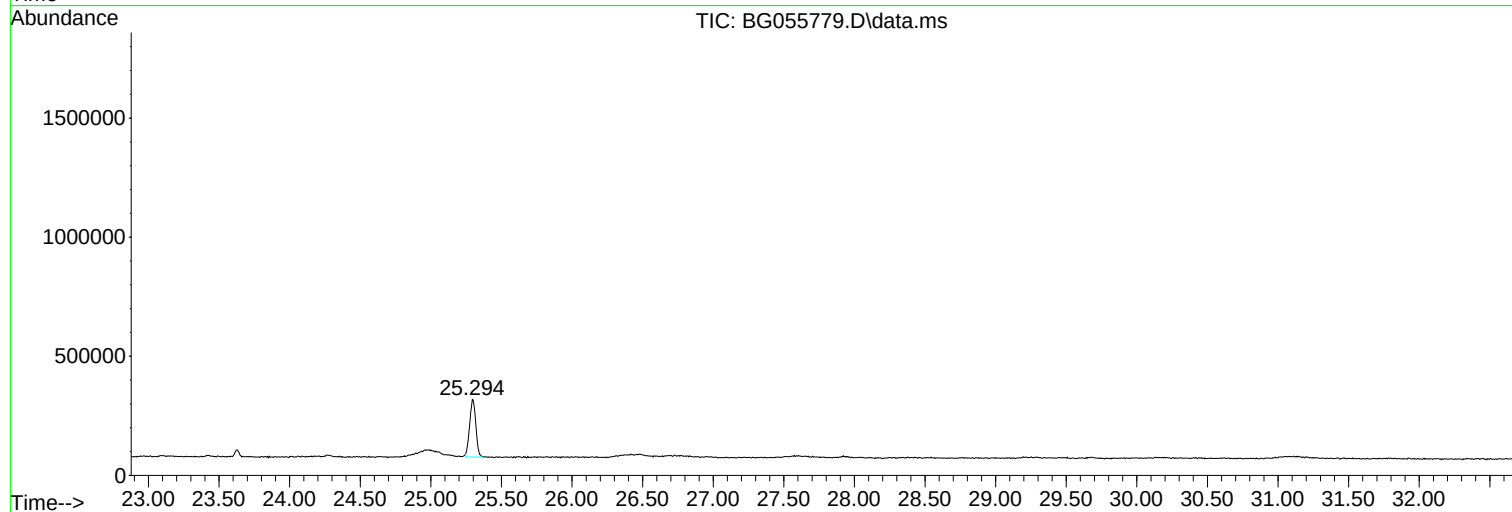
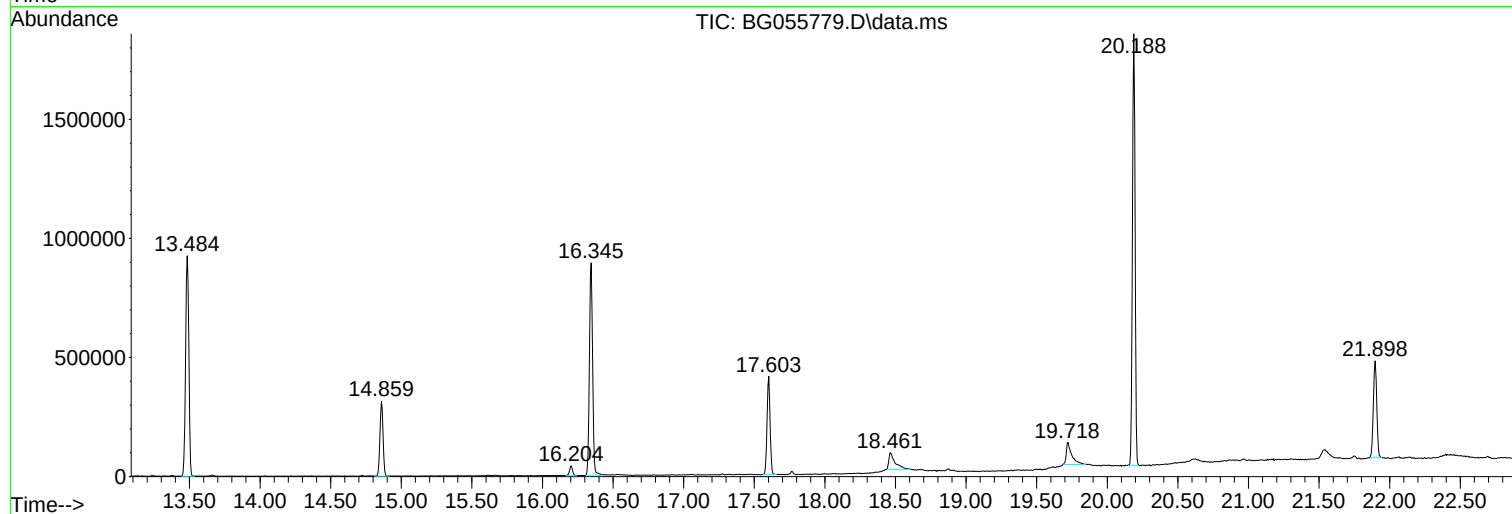
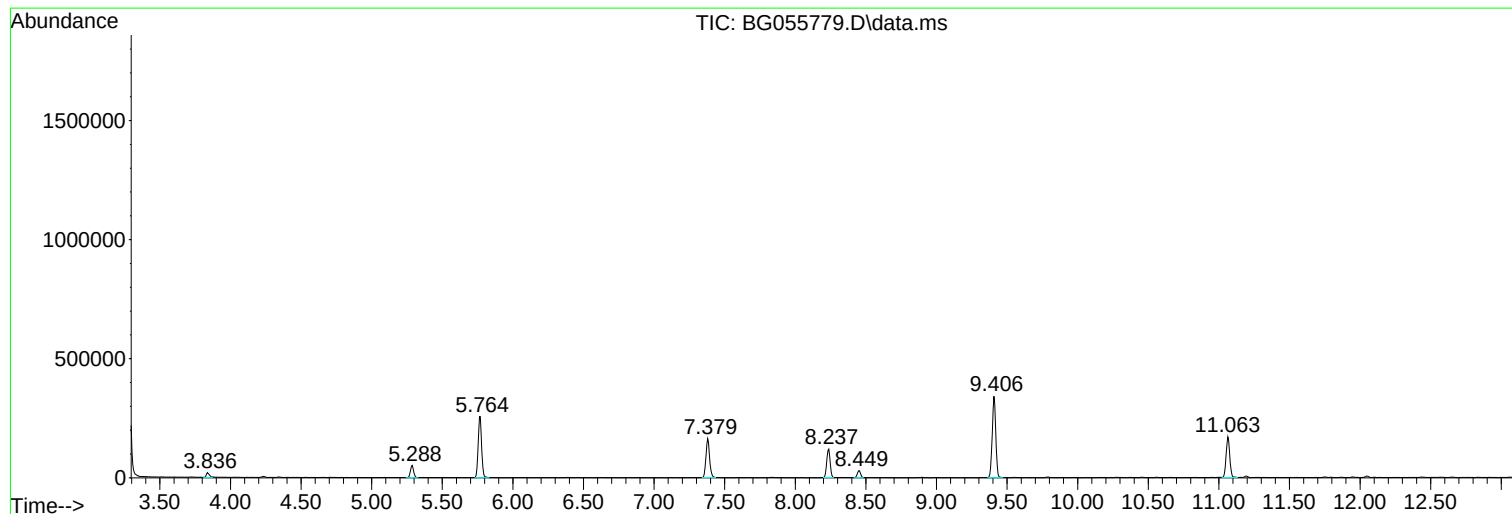
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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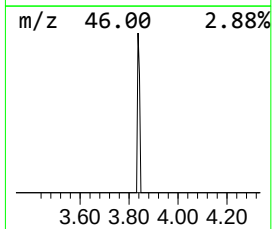
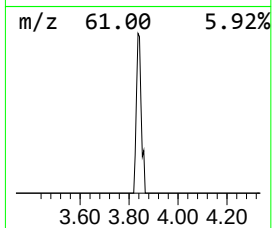
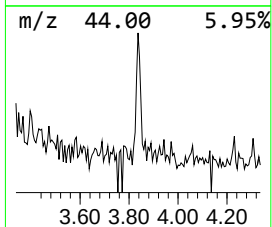
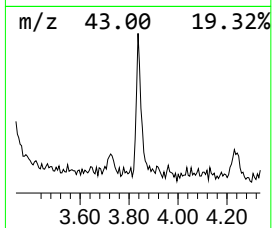
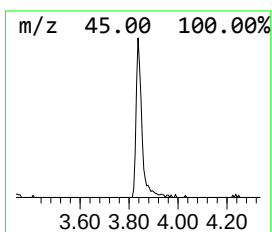
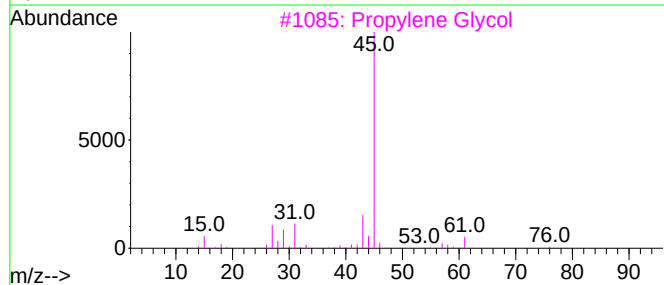
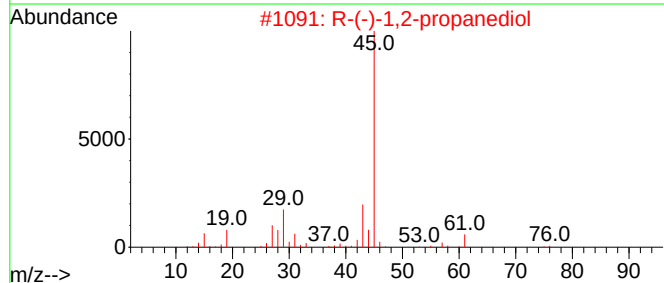
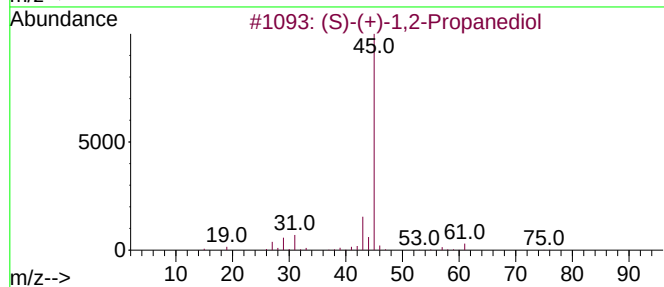
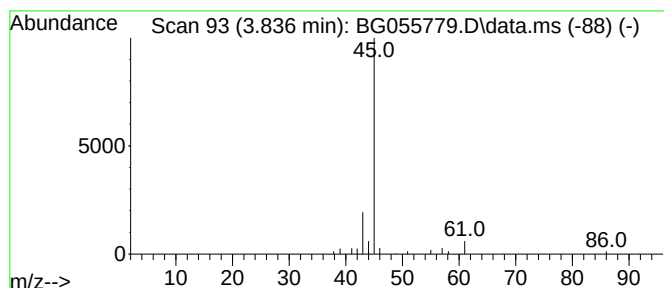
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 (S)-(+)-1,2-Propanediol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.836	2.91 ng	29164	1,4-Dichlorobenzene-d4	8.237

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-1,2-Propanediol			76	C3H8O2	004254-15-3	64
2	R-(-)-1,2-propanediol			76	C3H8O2	004254-14-2	43
3	Propylene Glycol			76	C3H8O2	000057-55-6	40
4	1-Butene, 4-methoxy			86	C5H10O	004696-30-4	9
5	2-Butanol			74	C4H10O	000078-92-2	9



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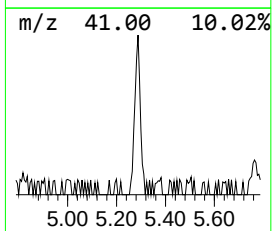
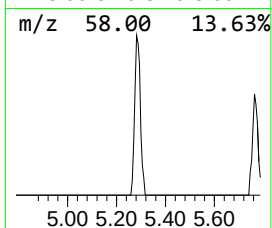
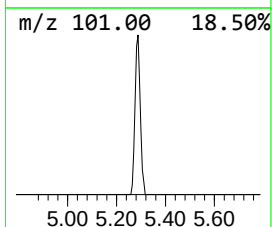
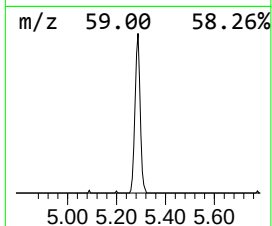
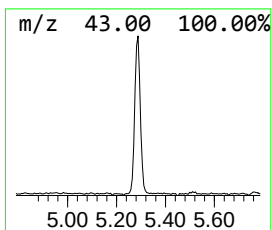
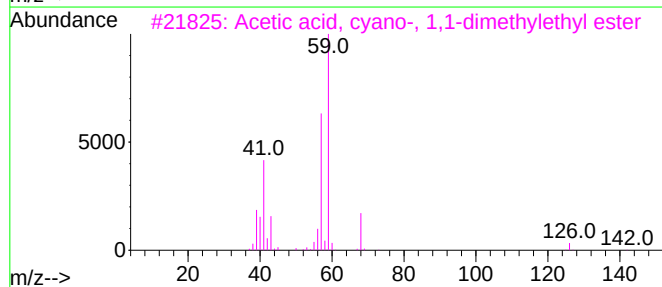
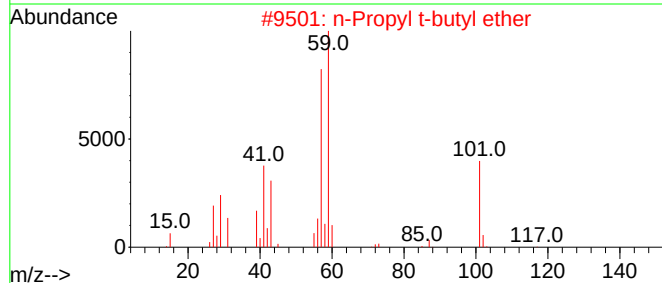
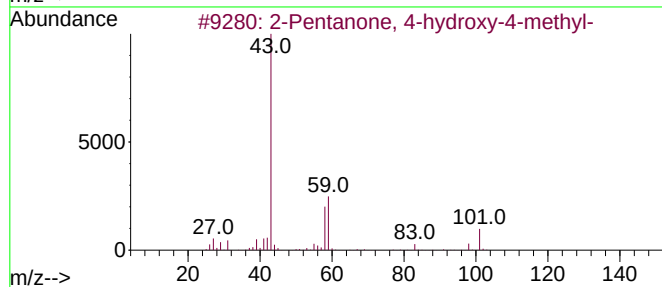
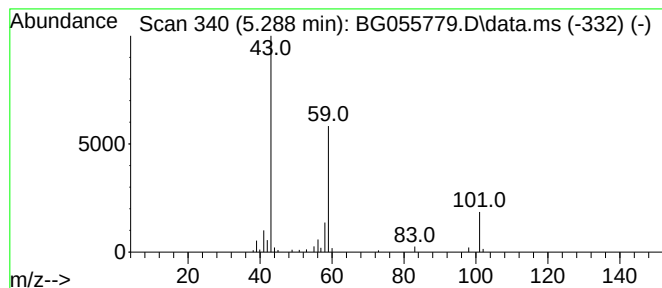
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.288	8.07 ng	80932	1,4-Dichlorobenzene-d4	8.237

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	33
3		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
4		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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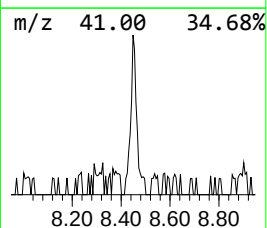
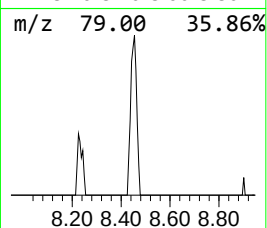
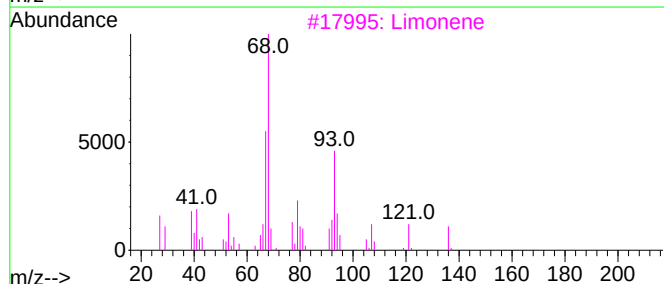
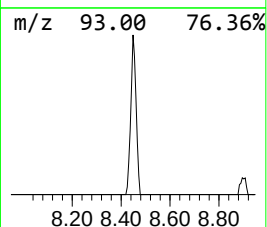
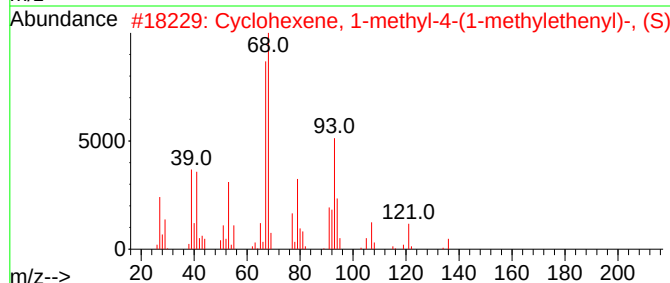
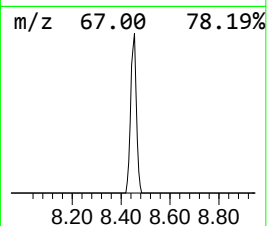
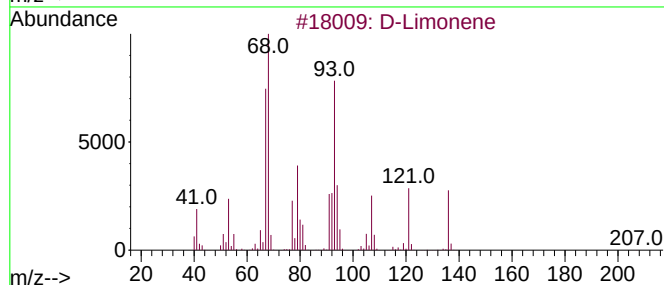
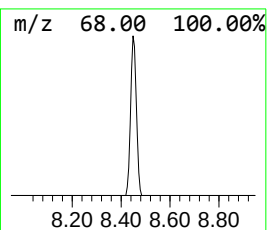
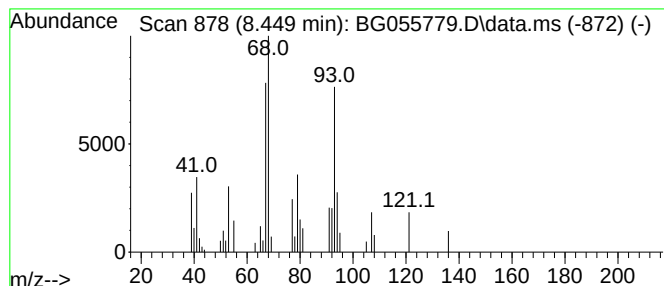
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Peak Number 3 D-Limonene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.449	4.75 ng	47597	1,4-Dichlorobenzene-d4	8.237

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			D-Limonene	136	C10H16	005989-27-5	98
2			Cyclohexene, 1-methyl-4-(1-methy...	136	C10H16	005989-54-8	94
3			Limonene	136	C10H16	000138-86-3	94
4			Cyclohexene, 1-methyl-5-(1-methy...	136	C10H16	013898-73-2	86
5			Cyclohexene, 4-ethenyl-1,4-dimet...	136	C10H16	001743-61-9	43



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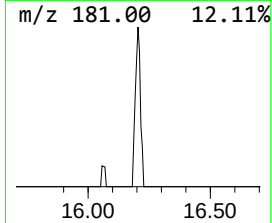
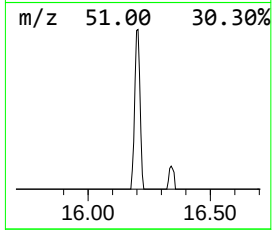
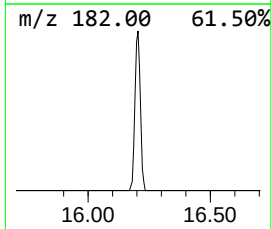
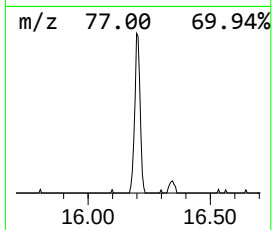
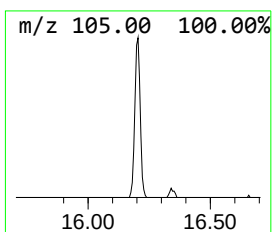
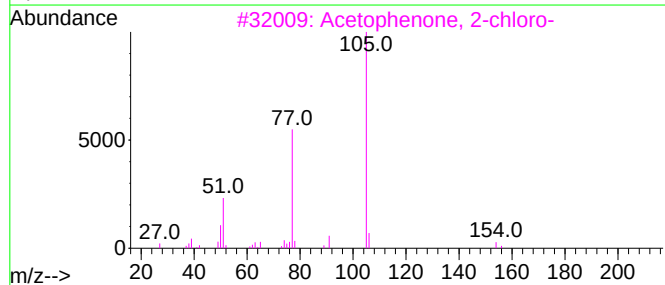
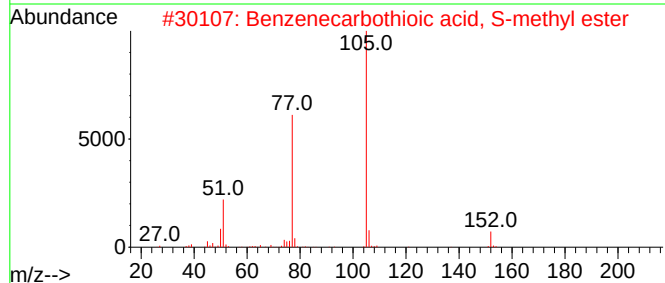
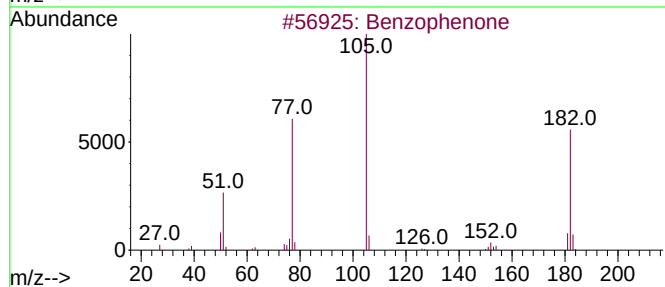
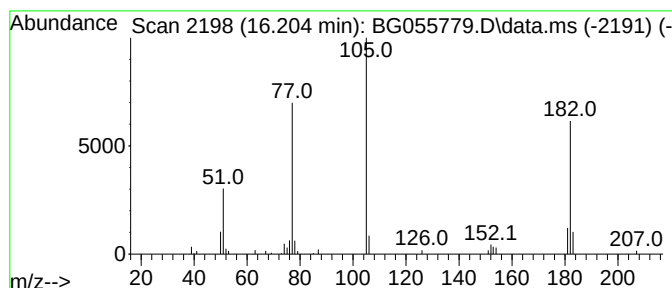
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Peak Number 4 Benzophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.204	2.74 ng	64935	Acenaphthene-d10	14.859

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	53
3			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
4			N-(1-Cyanovinyl)benzamide	172	C10H8N2O	1000186-19-1	47
5			2-Pyrazoline-3-carbonitrile, 1-b...	199	C11H9N3O	067872-68-8	47



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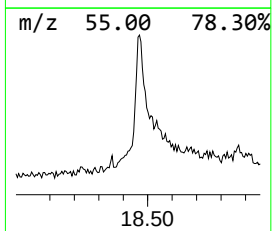
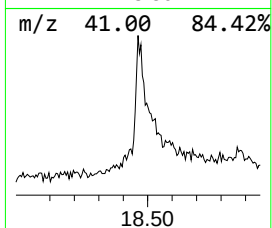
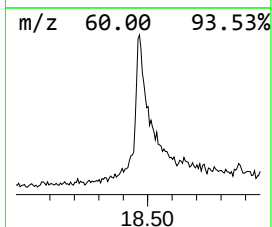
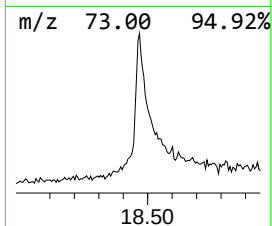
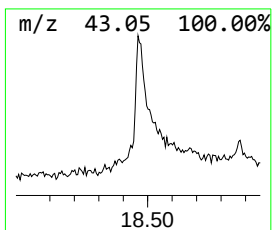
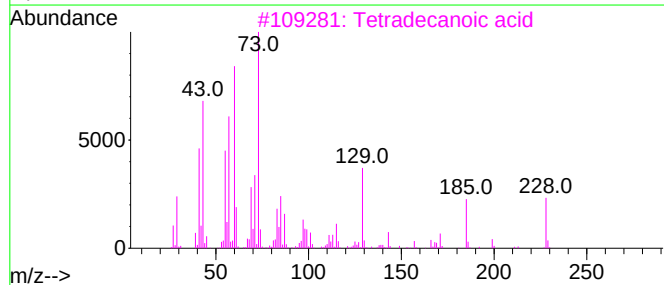
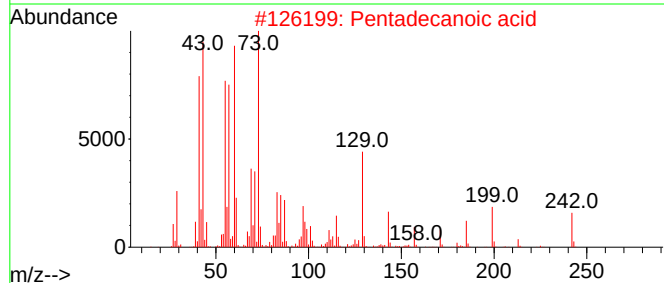
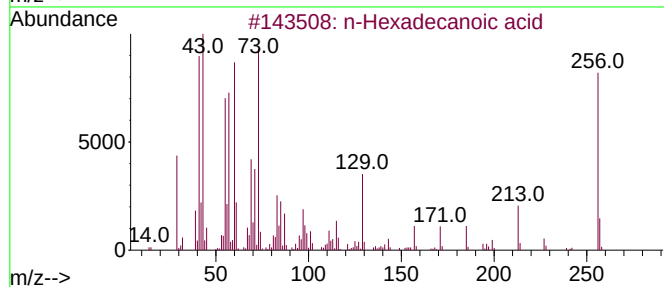
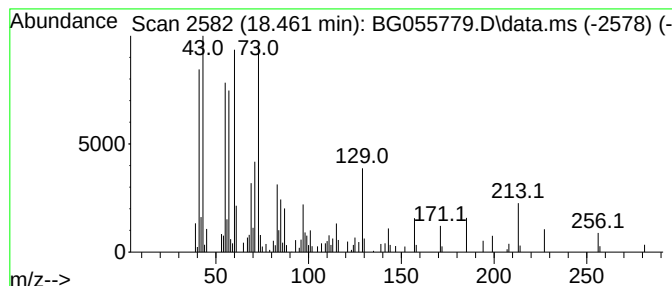
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.461	7.32 ng	227590	Phenanthrene-d10	17.603

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4			n-Decanoic acid	172	C10H20O2	000334-48-5	76
5			Tridecanoic acid	214	C13H26O2	000638-53-9	38



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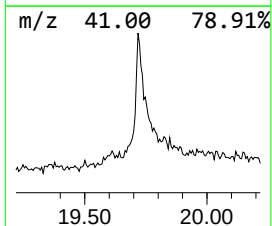
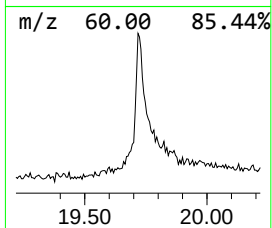
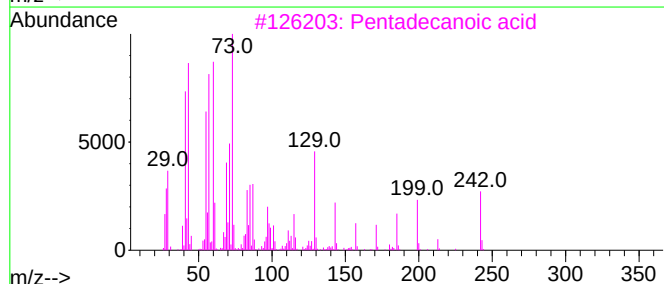
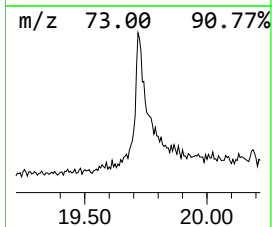
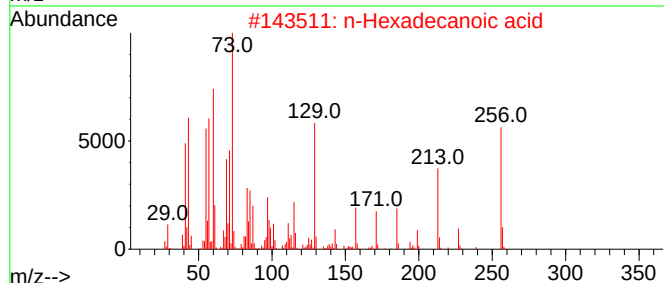
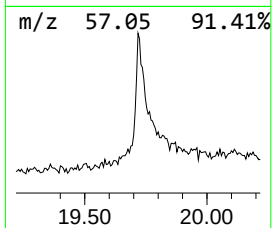
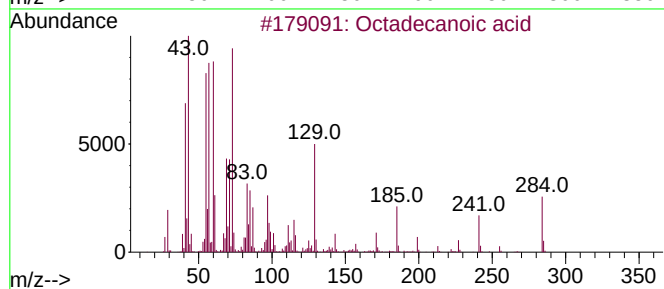
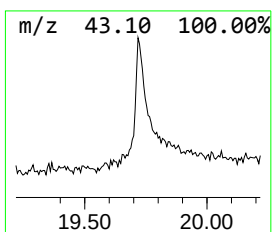
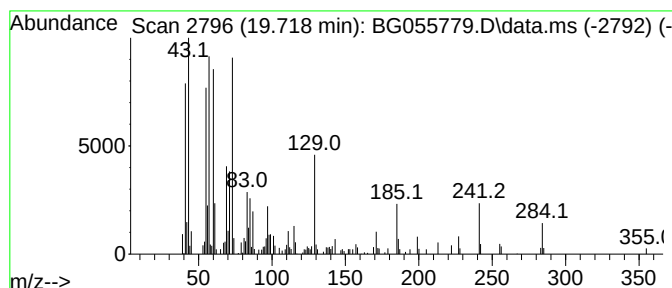
Instrument :
BNA_G
ClientSampleId :
MW-15

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG11622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.718	7.83 ng	243630	Phenanthrene-d10	17.603	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	89
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5	n-Decanoic acid	172	C10H20O2	000334-48-5	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112522\
Data File : BG055779.D
Acq On : 25 Nov 2022 13:36
Operator : CG/JU
Sample : N5741-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-15

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(S)-(+)-1,2-Pro...	3.836	2.9	ng	29164	1	8.237	200541	20.0
2-Pentanone, 4-...	5.288	8.1	ng	80932	1	8.237	200541	20.0
D-Limonene	8.449	4.8	ng	47597	1	8.237	200541	20.0
Benzophenone	16.204	2.7	ng	64935	3	14.859	474125	20.0
n-Hexadecanoic ...	18.461	7.3	ng	227590	4	17.603	621930	20.0
Octadecanoic acid	19.718	7.8	ng	243630	4	17.603	621930	20.0