

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100920\
 Data File : BG046838.D
 Acq On : 9 Oct 2020 17:43
 Operator : CG/JU
 Sample : L4233-01
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 55-ST-29

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-BG092220.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG046838.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.665	389	396	407	rBV	398401	618169	11.12%	2.874%
2	7.251	658	666	674	rBV	250166	414550	7.45%	1.928%
3	8.103	805	811	820	rVB	248747	421505	7.58%	1.960%
4	8.432	859	867	874	rVB	1036898	1748233	31.44%	8.129%
5	9.267	1002	1009	1023	rVB	832197	1492422	26.84%	6.940%
6	9.690	1076	1081	1092	rVB5	27309	58844	1.06%	0.274%
7	10.424	1200	1206	1212	rVB2	62269	113212	2.04%	0.526%
8	10.630	1228	1241	1243	rBV7	45710	133339	2.40%	0.620%
9	10.683	1245	1250	1254	rVV5	36455	59010	1.06%	0.274%
10	10.741	1254	1260	1265	rBV5	75264	164054	2.95%	0.763%
11	10.918	1283	1290	1297	rVB	283142	520871	9.37%	2.422%
12	11.088	1310	1319	1328	rVB9	27890	69131	1.24%	0.321%
13	11.188	1328	1336	1345	rBV6	27346	68301	1.23%	0.318%
14	11.746	1428	1431	1439	rVB3	41072	81786	1.47%	0.380%
15	11.870	1448	1452	1456	rVV2	41392	60123	1.08%	0.280%
16	11.922	1456	1461	1469	rVB5	32599	67567	1.22%	0.314%
17	13.356	1696	1705	1714	rBV	2037783	3204856	57.63%	14.902%
18	14.725	1933	1938	1947	rVB2	478570	768718	13.82%	3.574%
19	16.212	2184	2191	2198	rBV2	1131265	1745813	31.39%	8.118%
20	17.469	2399	2405	2415	rBV	621098	990005	17.80%	4.603%
21	18.350	2550	2555	2562	rBV2	129419	193971	3.49%	0.902%
22	18.562	2587	2591	2597	rBV2	56859	76854	1.38%	0.357%
23	19.613	2767	2770	2778	rBV4	73346	115951	2.09%	0.539%
24	19.766	2791	2796	2801	rVB3	41804	71369	1.28%	0.332%
25	20.078	2842	2849	2856	rBV	4180355	5560955	100.00%	25.858%
26	21.388	3068	3072	3080	rBV5	65471	132014	2.37%	0.614%
27	21.740	3126	3132	3141	rVB	742151	1265233	22.75%	5.883%
28	25.007	3677	3688	3702	rBV2	430367	1288921	23.18%	5.993%

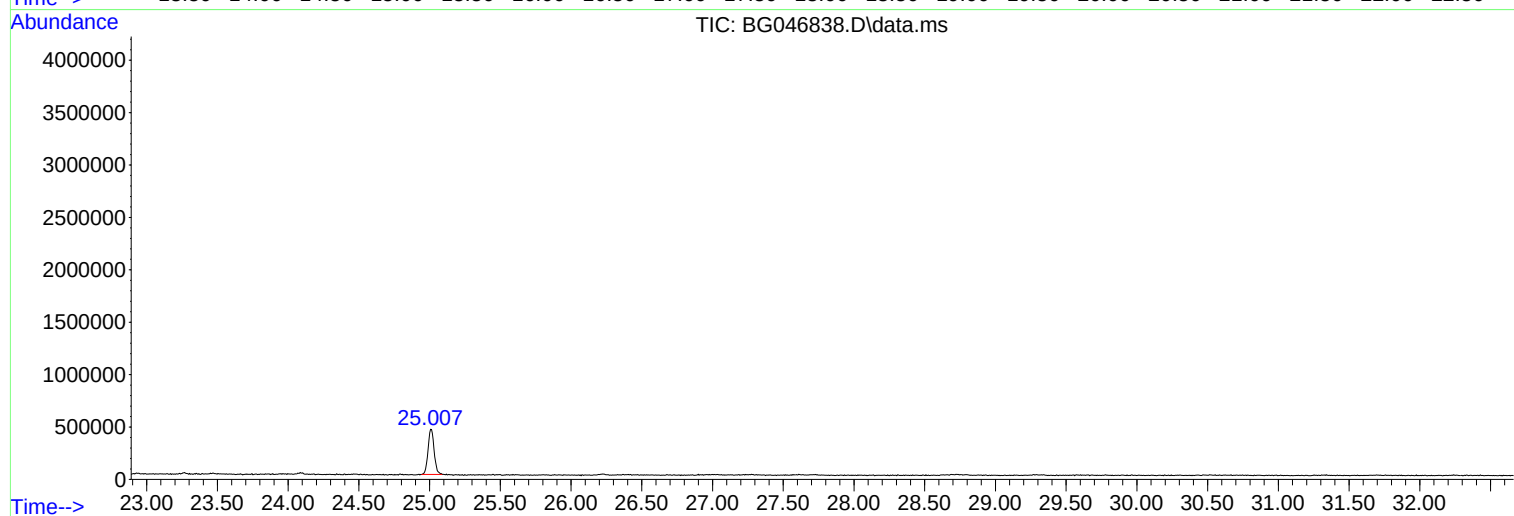
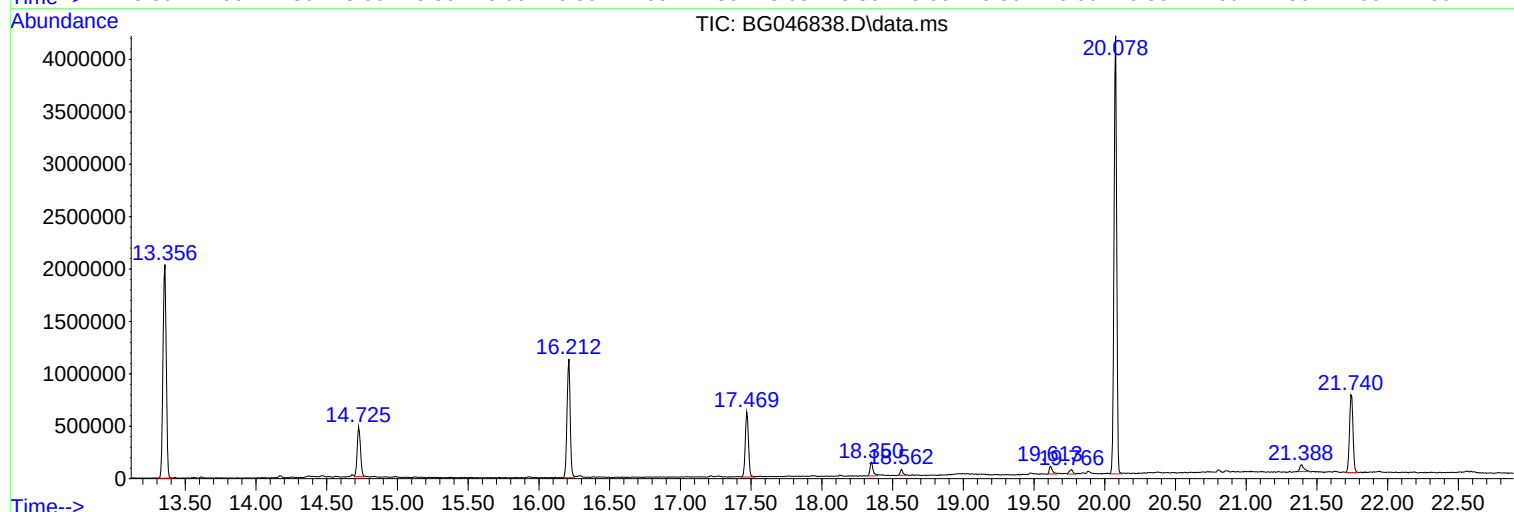
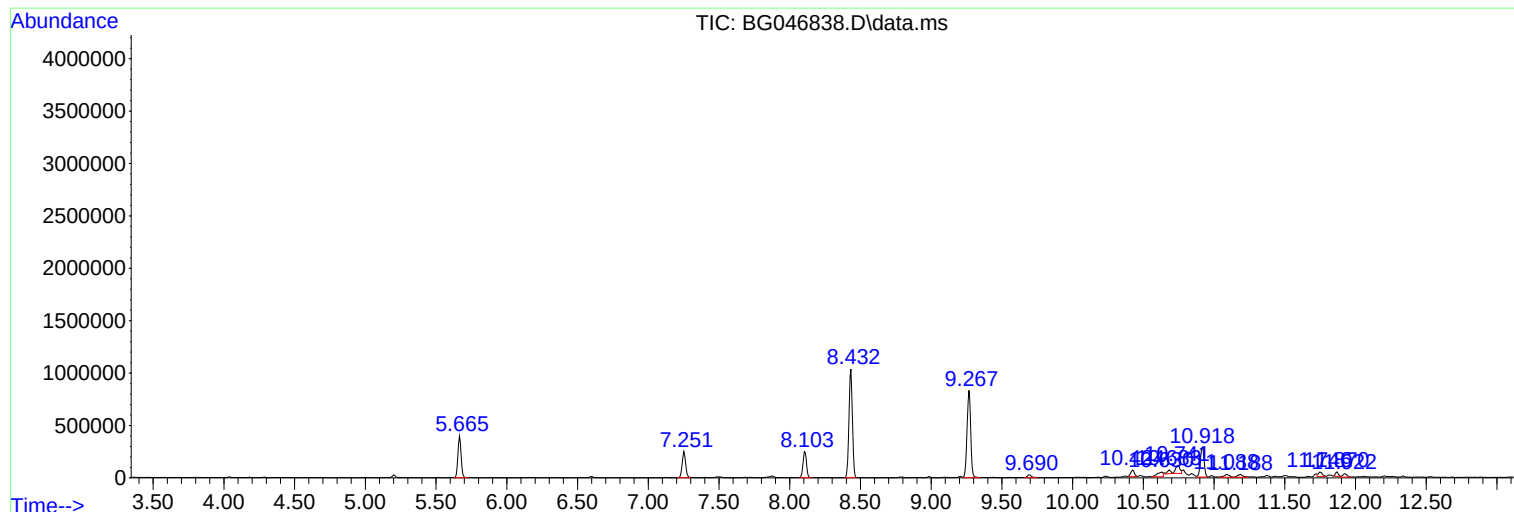
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Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



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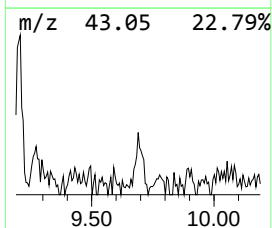
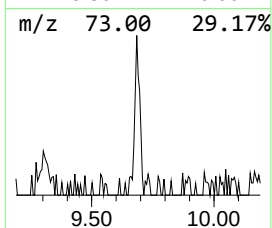
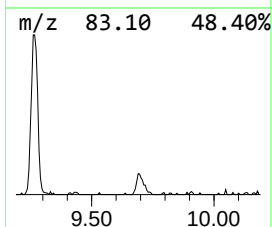
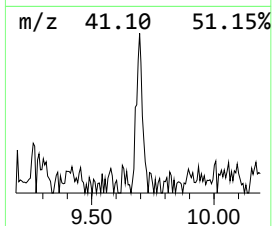
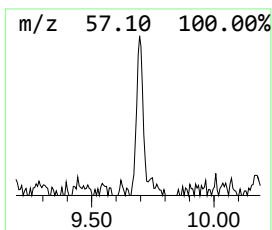
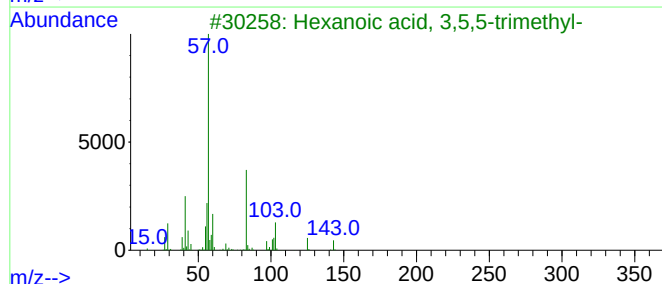
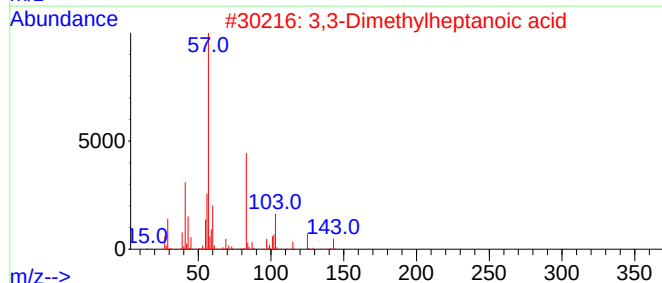
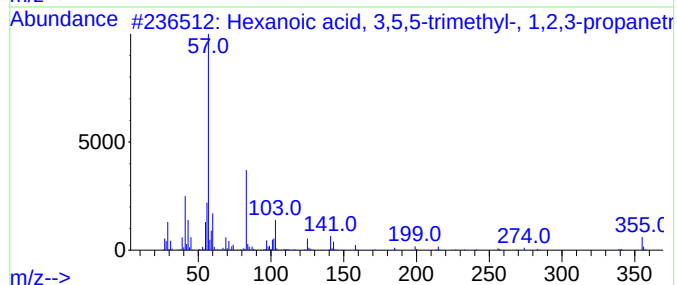
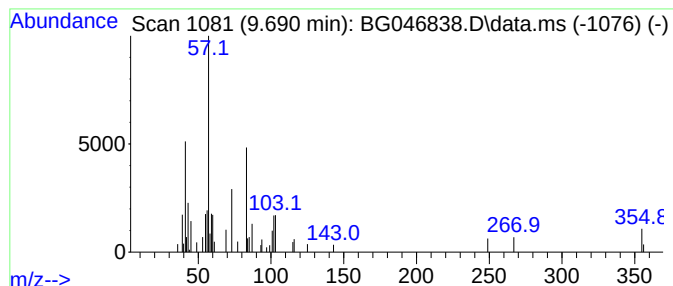
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown9.69 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.690	2.26 ng	58844	Naphthalene-d8	10.918

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanoic acid, 3,5,5-trimethyl-,...	512	C30H56O6	056554-53-1	42
2			3,3-Dimethylheptanoic acid	158	C9H18O2	067061-30-7	38
3			Hexanoic acid, 3,5,5-trimethyl-	158	C9H18O2	003302-10-1	38
4			Hexanal, 3,5,5-trimethyl-	142	C9H18O	005435-64-3	14
5			4,4-Dimethyl-2-pentanol, chlorod...	228	C9H15ClF2O2	1000376-27-0	14



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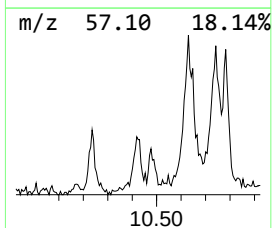
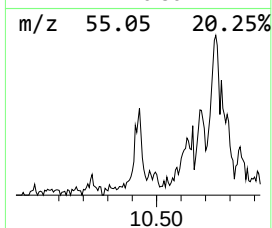
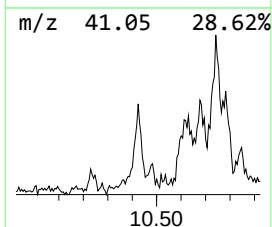
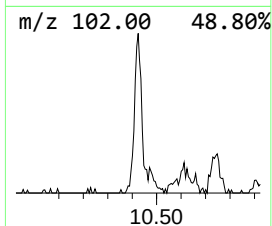
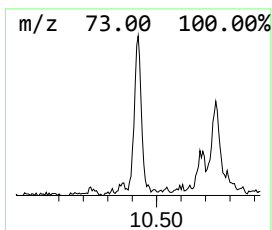
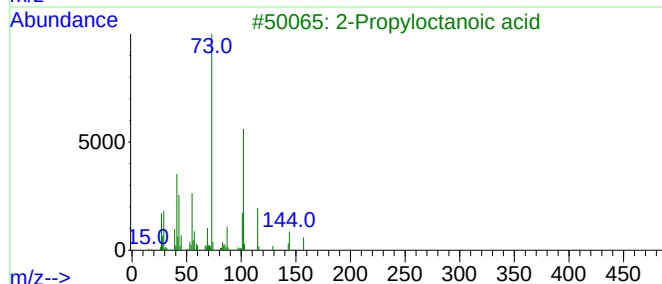
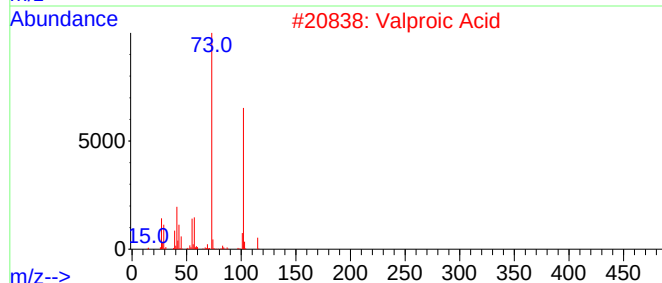
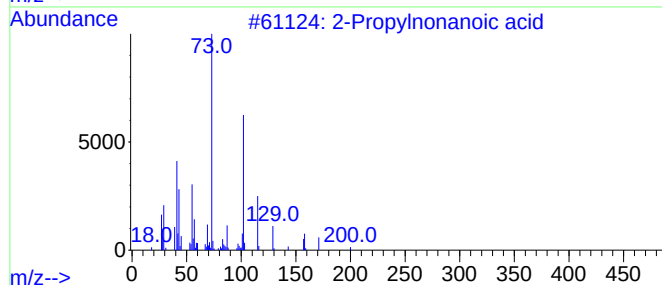
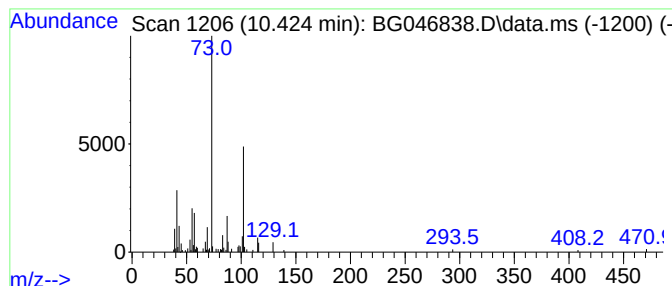
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Propylnonanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.424	4.35 ng	113212	Naphthalene-d8	10.918

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Propylnonanoic acid	200	C12H24O2	065185-82-2	56
2			Valproic Acid	144	C8H16O2	000099-66-1	43
3			2-Propyloctanoic acid	186	C11H22O2	031080-41-8	39
4			di-n-Propylmalonic acid	188	C9H16O4	001636-27-7	25
5			.alpha.-D-Mannofuranoside, 1-O-h...	278	C13H26O6	111570-47-9	12



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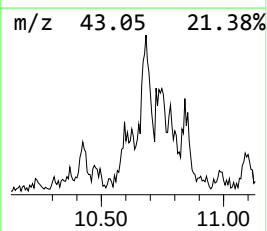
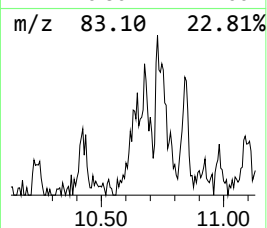
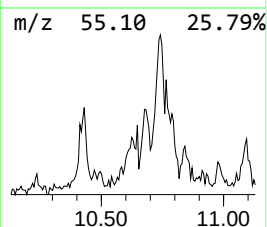
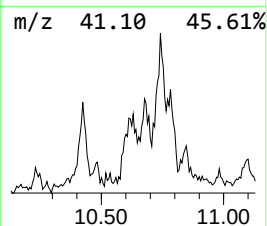
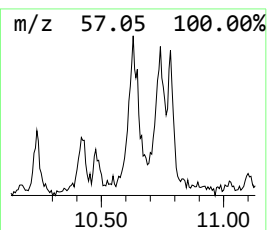
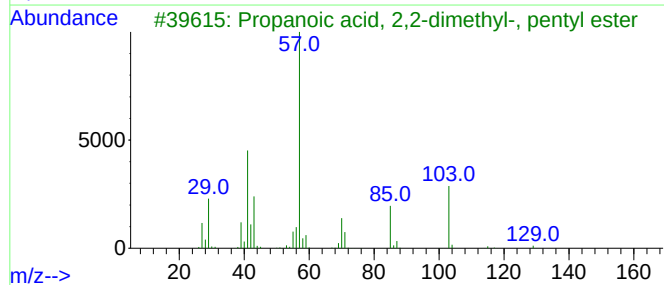
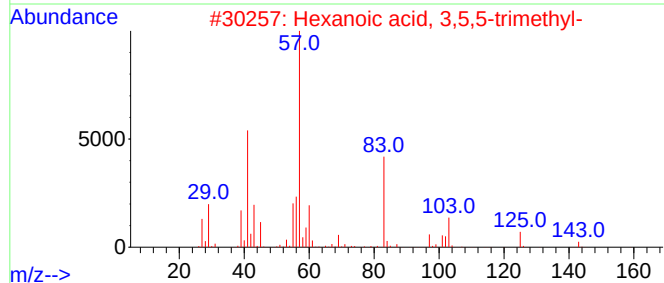
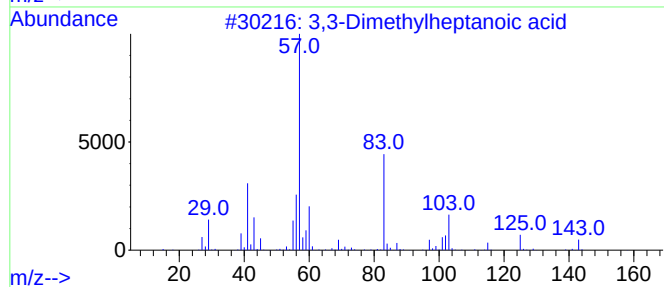
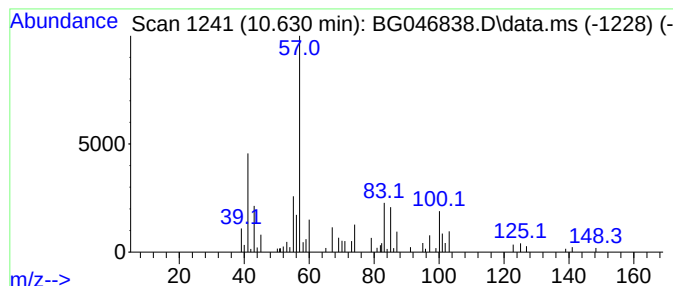
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown10.63 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.630	5.12 ng	133339	Naphthalene-d8	10.918

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3,3-Dimethylheptanoic acid	158	C9H18O2	067061-30-7	43
2			Hexanoic acid, 3,5,5-trimethyl-	158	C9H18O2	003302-10-1	38
3			Propanoic acid, 2,2-dimethyl-, p...	172	C10H20O2	002313-68-0	35
4			Propanoic acid, 2,2-dimethyl-, b...	158	C9H18O2	005129-37-3	35
5			Propanoic acid, 2,2-dimethyl-, h...	186	C11H22O2	005434-57-1	35



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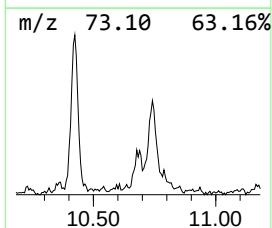
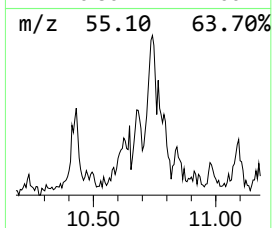
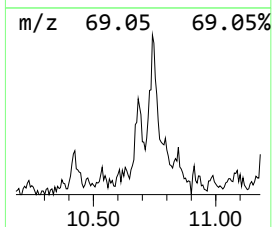
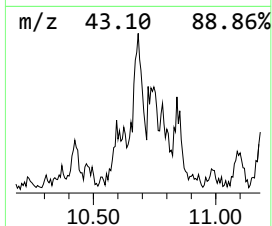
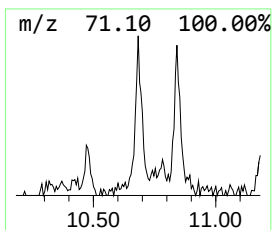
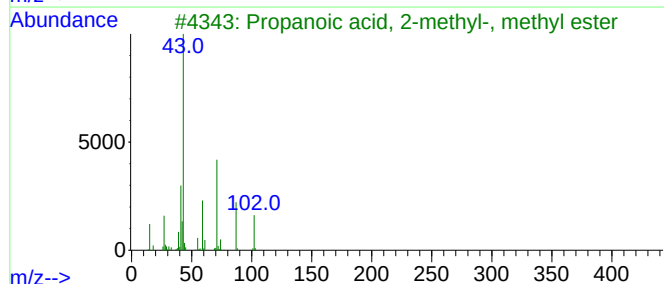
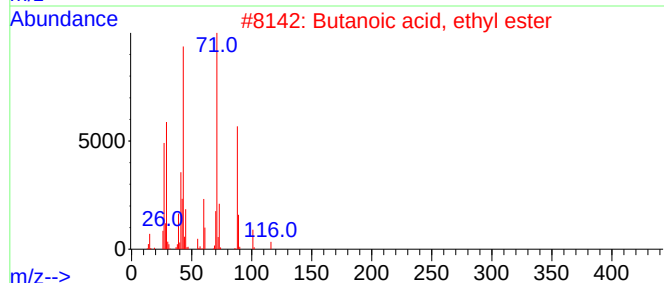
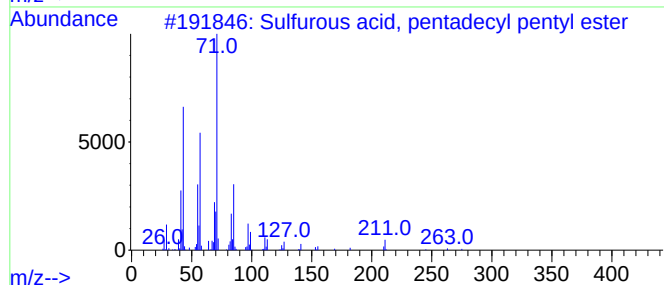
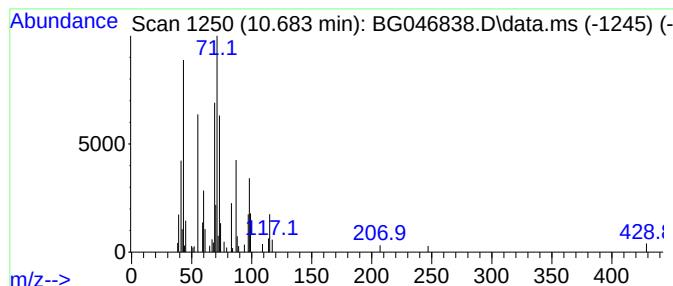
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TIC Library : C:\Database\NIST11.L
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Peak Number 5 unknown10.68 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.683	2.27 ng	59010	Naphthalene-d8	10.918

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, pentadecyl penty...	362	C20H42O3S	1000309-14-8	43
2			Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	43
3			Propanoic acid, 2-methyl-, methy...	102	C5H10O2	000547-63-7	37
4			Propionic acid, 2,2-dichloro-, p...	212	C8H14Cl2O2	017640-08-3	35
5			Cyclohexanol, 1-methyl-	114	C7H14O	000590-67-0	25



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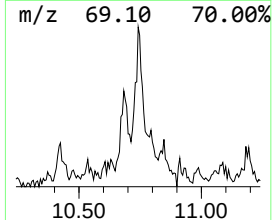
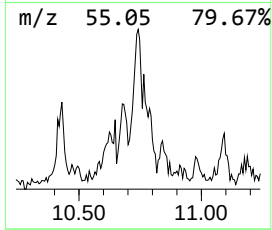
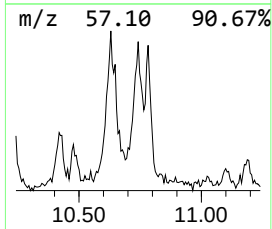
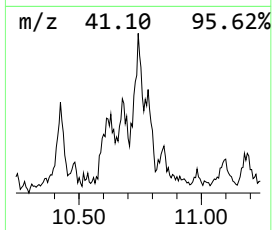
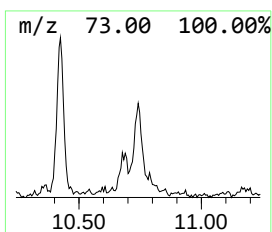
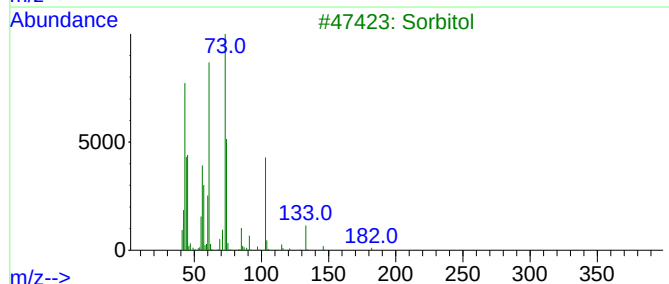
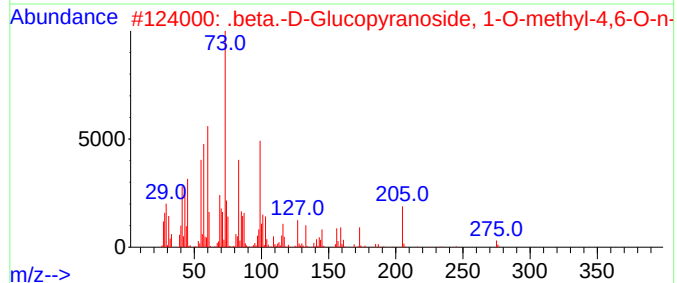
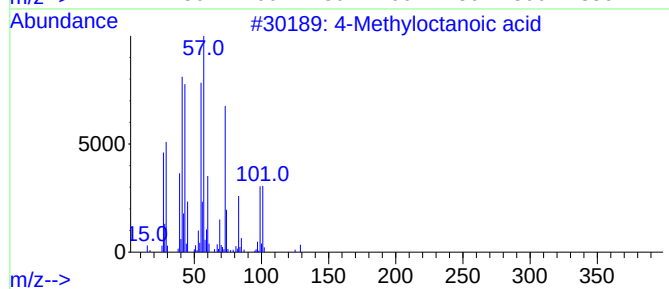
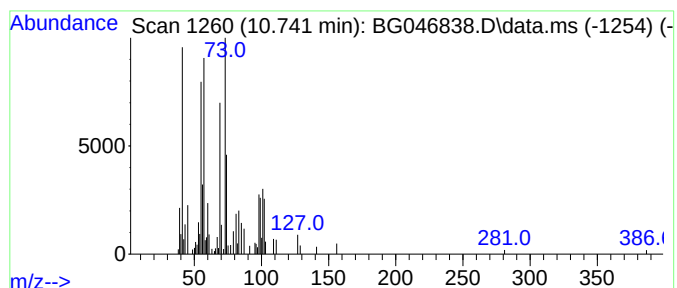
Instrument :
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown10.74 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.742	6.30 ng	164054	Naphthalene-d8	10.918	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Methyloctanoic acid	158	C9H18O2	054947-74-9	35
2	.beta.-D-Glucopyranoside, 1-O-me...	276	C13H24O6	1000160-64-2	35
3	Sorbitol	182	C6H14O6	000050-70-4	25
4	Formic acid, 2-methylhex-3-yl ester	144	C8H16O2	1000368-35-0	16
5	Azacyclotridecan-2-one	197	C12H23NO	000947-04-6	16



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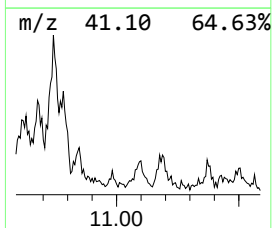
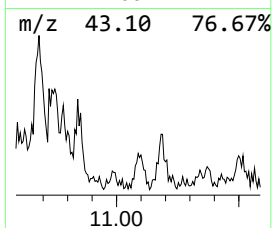
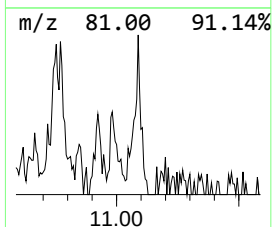
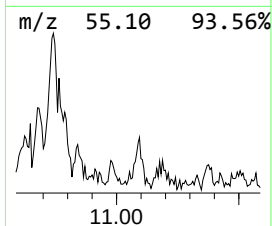
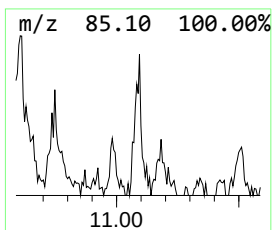
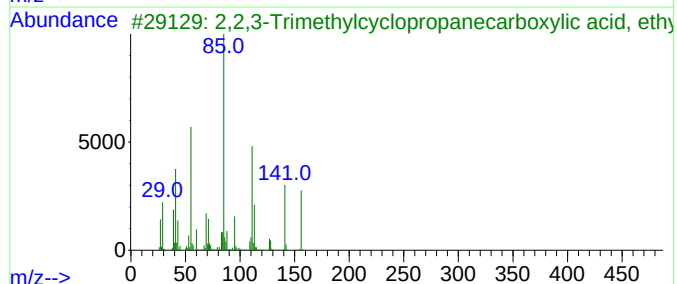
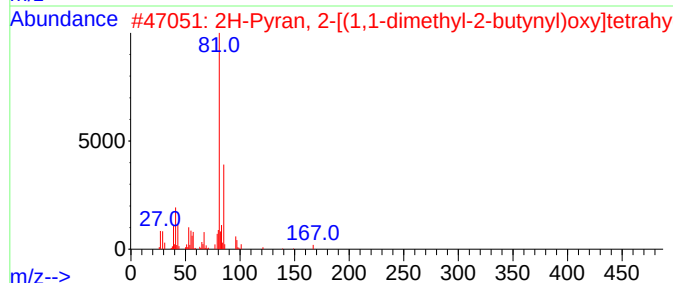
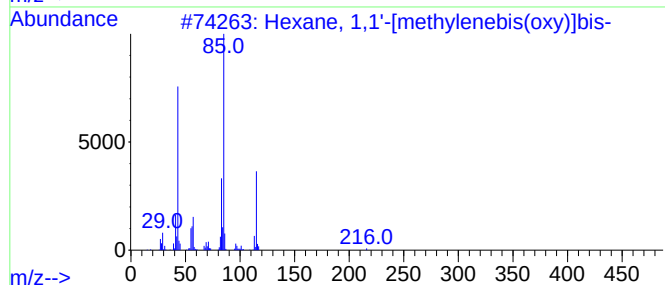
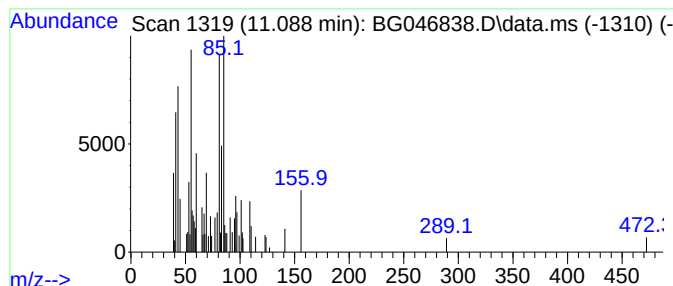
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 unknown11.08 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.088	2.65 ng	69131	Naphthalene-d8	10.918

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 1,1'-[methylenebis(oxy)]...	216	C13H28O2	054815-12-2	22		
2	2H-Pyran, 2-[(1,1-dimethyl-2-but...	182	C11H18O2	024642-03-3	22		
3	2,2,3-Trimethylcyclopropanecarbo...	156	C9H16O2	1000191-75-2	22		
4	1,4-Hexadiene, 4-methyl-	96	C7H12	001116-90-1	20		
5	2,4-Hexadiene, 3-methyl-	96	C7H12	028823-42-9	18		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100920\
Data File : BG046838.D
Acq On : 9 Oct 2020 17:43
Operator : CG/JU
Sample : L4233-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
55-ST-29

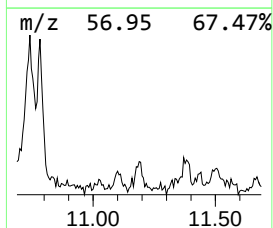
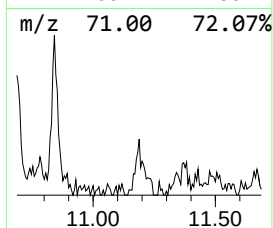
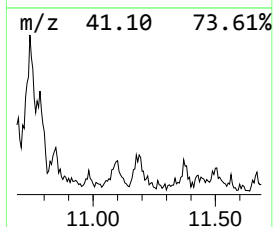
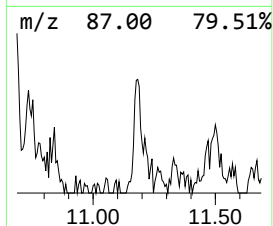
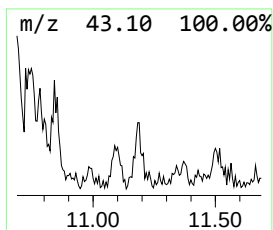
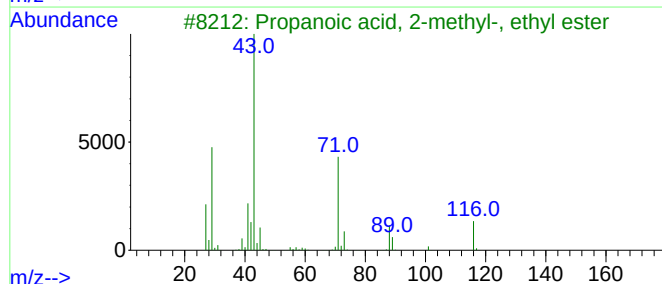
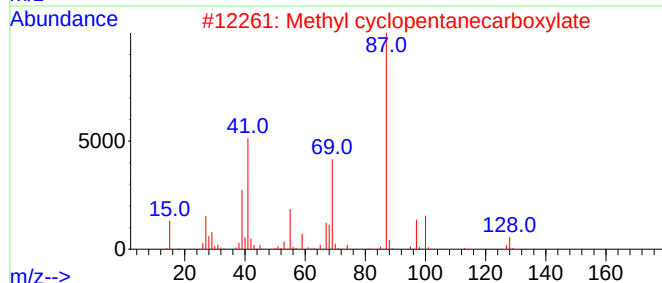
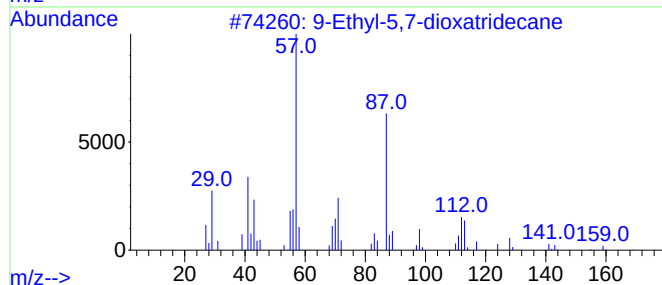
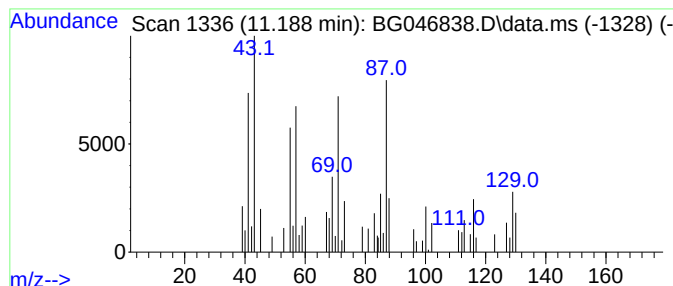
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 unknown11.18 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.188	2.62 ng	68301	Naphthalene-d8	10.918

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Ethyl-5,7-dioxatridecane	216	C13H28O2	1000334-82-6	27
2			Methyl cyclopentanecarboxylate	128	C7H12O2	004630-80-2	22
3			Propanoic acid, 2-methyl-, ethyl...	116	C6H12O2	000097-62-1	22
4			Z-1-Methoxy-2-pentene	100	C6H12O	1000279-59-4	11
5			Sulfurous acid, octyl 2-propyl e...	236	C11H24O3S	1000309-11-9	11



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100920\
Data File : BG046838.D
Acq On : 9 Oct 2020 17:43
Operator : CG/JU
Sample : L4233-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
55-ST-29

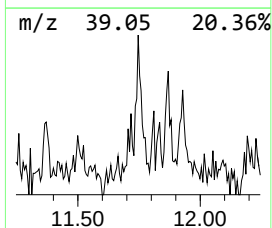
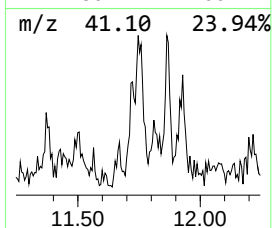
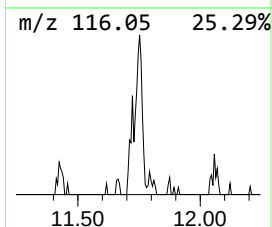
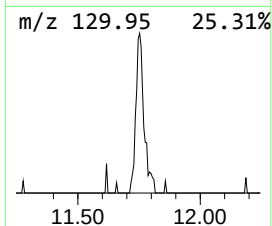
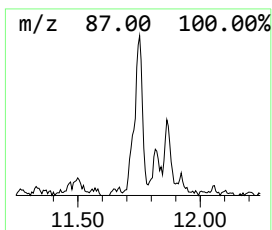
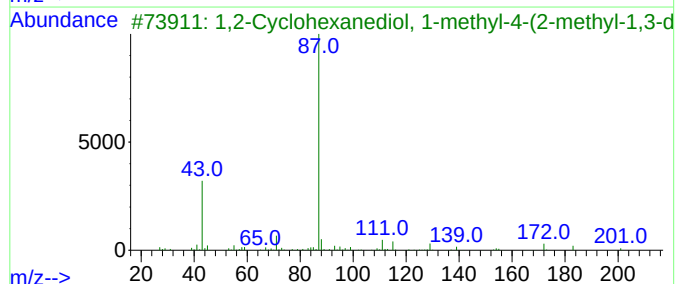
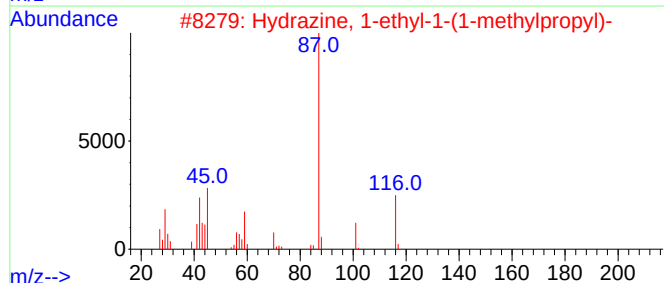
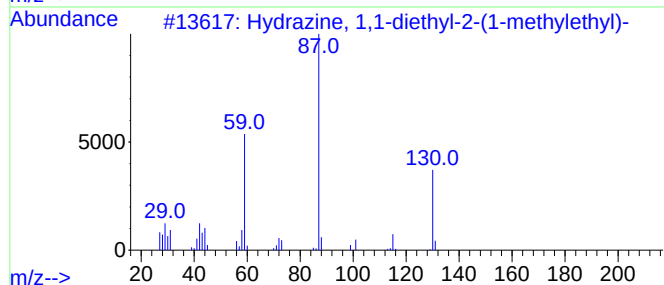
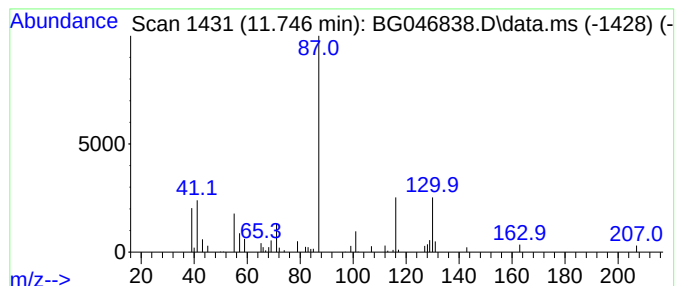
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 unknown11.76 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.746	3.14 ng	81786	Naphthalene-d8	10.918

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hydrazine, 1,1-diethyl-2-(1-meth...	130	C7H18N2	067398-39-4	42
2			Hydrazine, 1-ethyl-1-(1-methylpr...	116	C6H16N2	020325-97-7	40
3			1,2-Cyclohexanediol, 1-methyl-4-...	216	C11H20O4	056859-97-3	28
4			1,3-Dioxolane, 2-butyl-4-methyl-	144	C8H16O2	074094-60-3	25
5			1,3-Dioxolane-2-propanol, 2-meth...	188	C9H16O4	029021-95-2	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100920\
Data File : BG046838.D
Acq On : 9 Oct 2020 17:43
Operator : CG/JU
Sample : L4233-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
55-ST-29

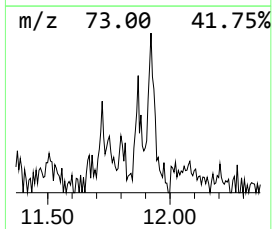
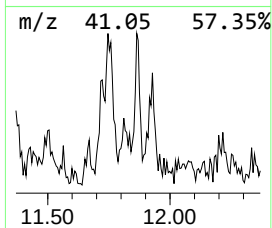
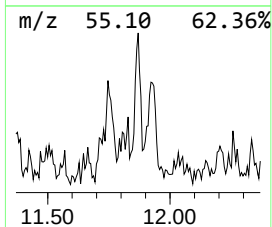
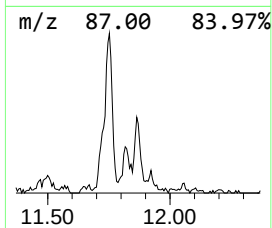
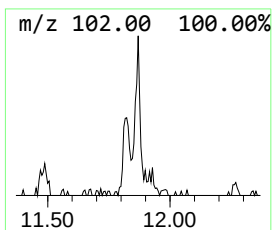
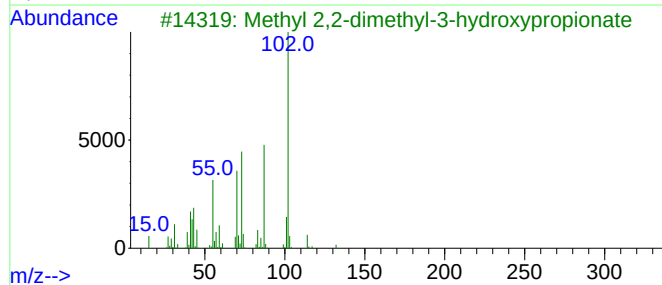
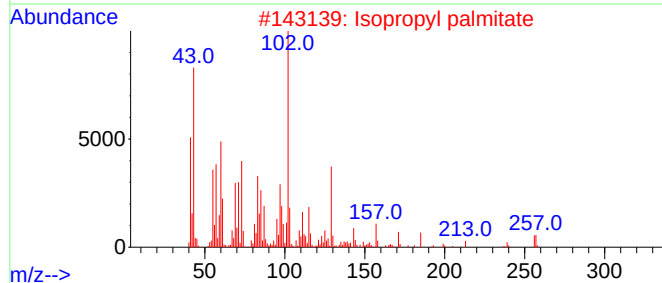
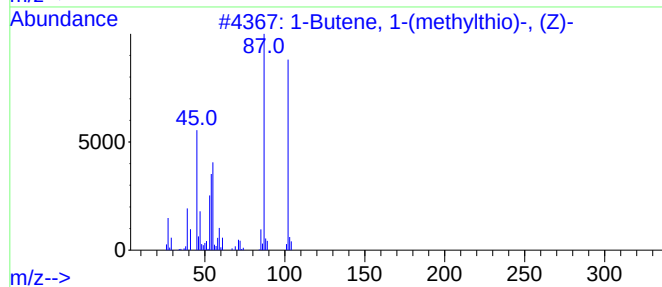
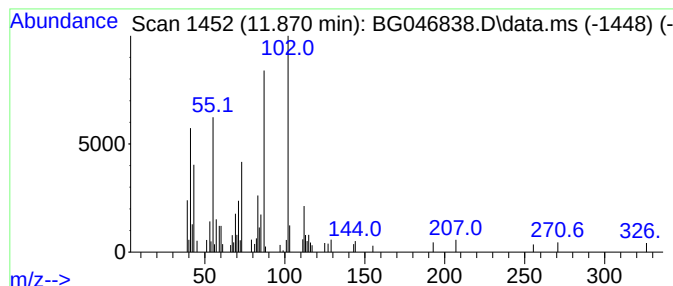
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 unknown11.87 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.870	2.31 ng	60123	Naphthalene-d8	10.918

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Butene, 1-(methylthio)-, (Z)-	102	C5H10S	017414-15-2	42
2			Isopropyl palmitate	298	C19H38O2	000142-91-6	38
3			Methyl 2,2-dimethyl-3-hydroxypro...	132	C6H12O3	014002-80-3	25
4			Aziridine-2-carbothioamide	102	C3H6N2S	1000189-98-7	25
5			l-Aspartic acid, N-isovaleryl-, ...	245	C11H19NO5	1000153-13-8	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100920\
Data File : BG046838.D
Acq On : 9 Oct 2020 17:43
Operator : CG/JU
Sample : L4233-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampled :
55-ST-29

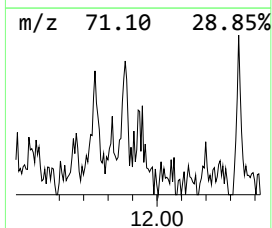
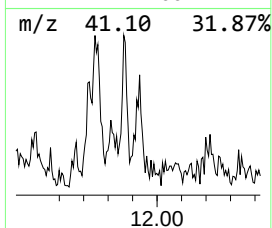
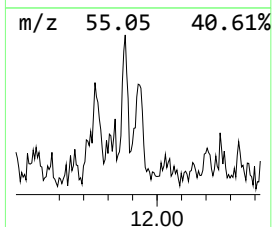
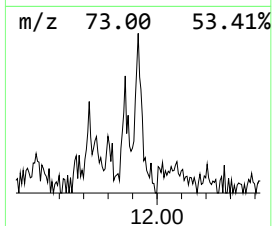
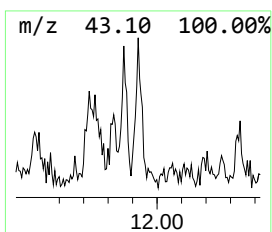
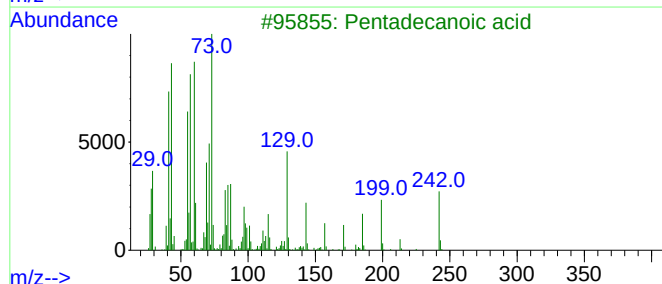
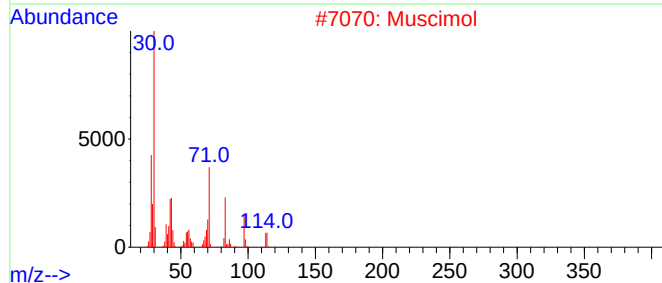
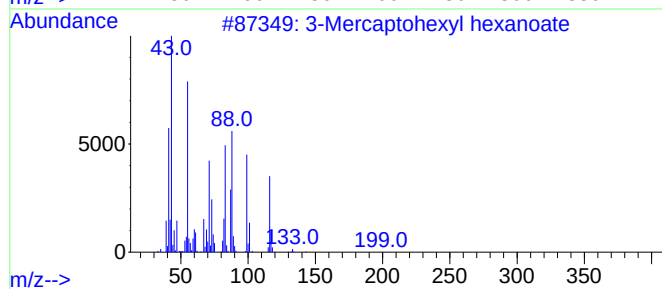
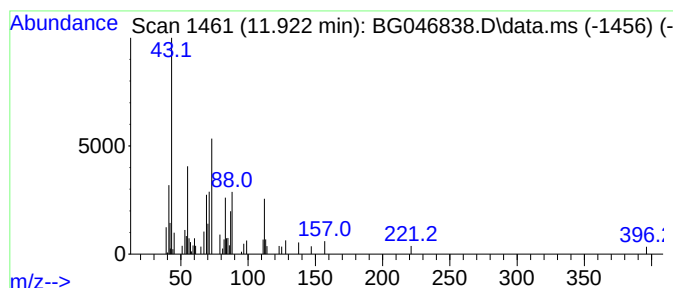
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 unknown11.92 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.922	2.59 ng	67567	Naphthalene-d8	10.918

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Mercaptohexyl hexanoate	232	C12H24O2S	136954-22-8	38
2			Muscimol	114	C4H6N2O2	002763-96-4	22
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	16
4			1,5-Dimethyl-6-oxa-bicyclo[3.1.0]...	112	C7H12O	082461-31-2	14
5			Dimethylmalonic acid, decyl 3-me...	342	C20H38O4	1000361-59-8	12



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100920\
Data File : BG046838.D
Acq On : 9 Oct 2020 17:43
Operator : CG/JU
Sample : L4233-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
55-ST-29

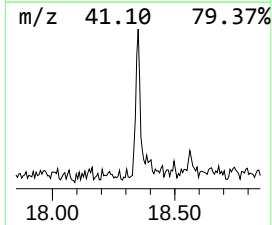
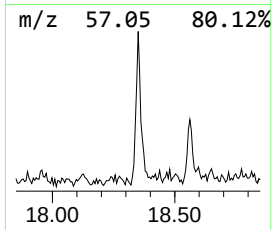
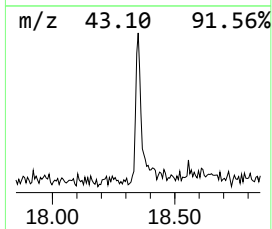
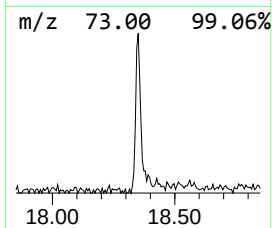
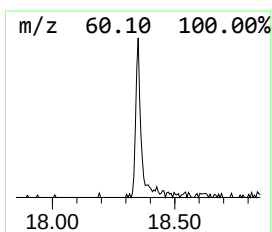
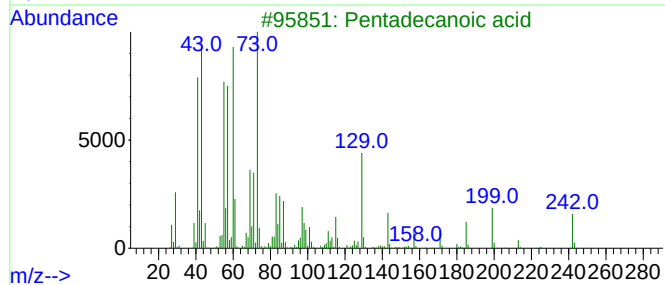
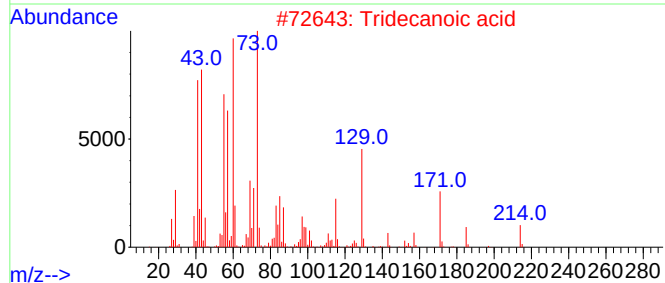
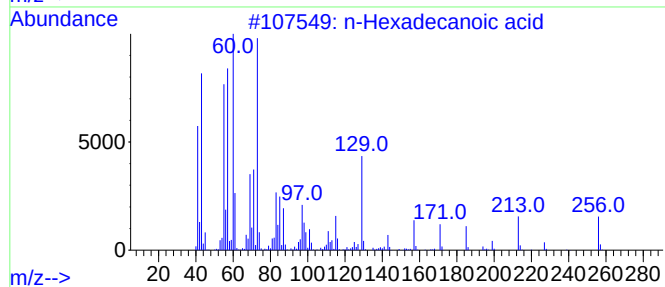
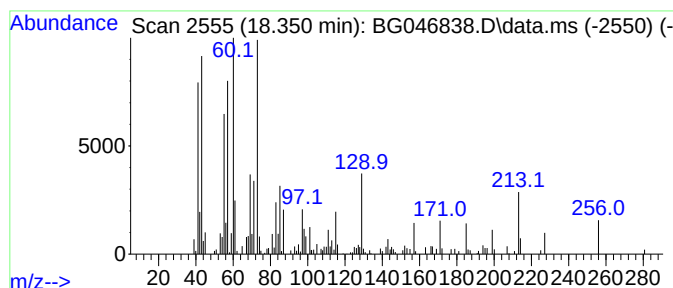
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.350	3.92 ng	193971	Phenanthrene-d10	17.469

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tridecanoic acid	214	C13H26O2	000638-53-9	94
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4		Dodecanoic acid	200	C12H24O2	000143-07-7	72
5		Tetradecanoic acid	228	C14H28O2	000544-63-8	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100920\
Data File : BG046838.D
Acq On : 9 Oct 2020 17:43
Operator : CG/JU
Sample : L4233-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
55-ST-29

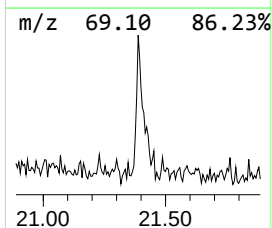
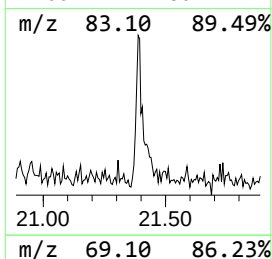
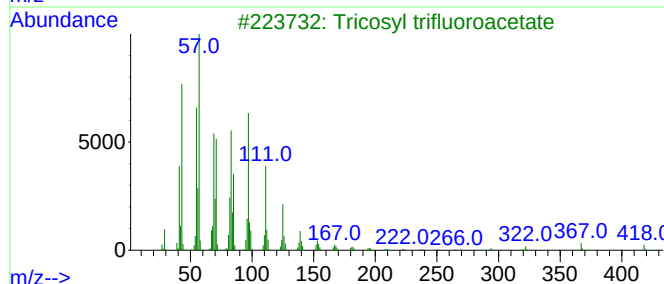
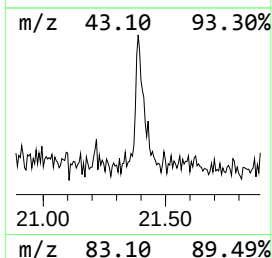
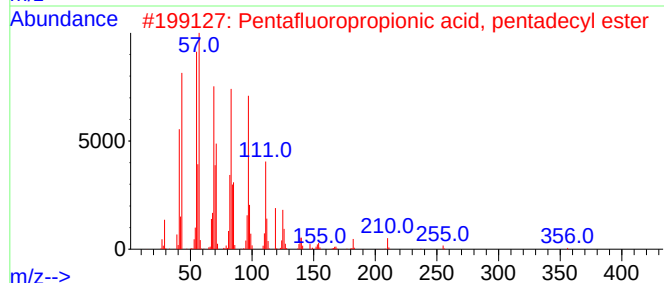
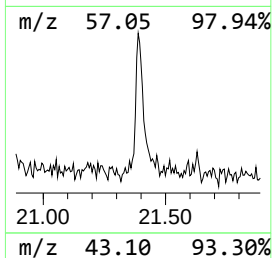
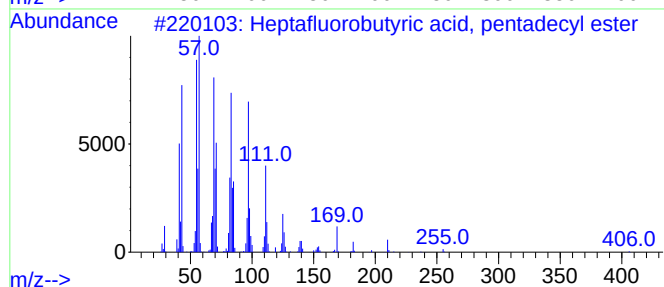
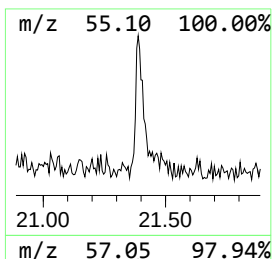
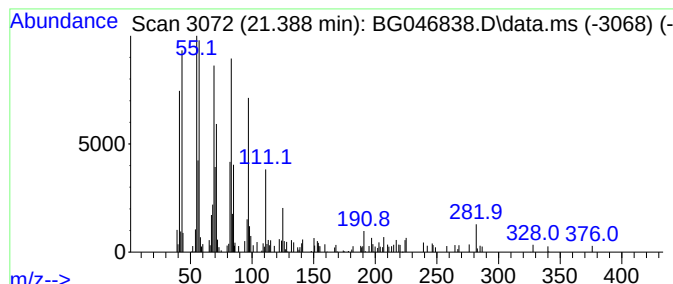
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 Heptafluorobutyric acid, pe... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.388	2.09 ng	132014	Chrysene-d12	21.740

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91
2			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91
3			Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	55
4			Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	53
5			Dotriacontyl heptafluorobutyrate	662	C36H65F7O2	1000351-84-2	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100920\
 Data File : BG046838.D
 Acq On : 9 Oct 2020 17:43
 Operator : CG/JU
 Sample : L4233-01
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 55-ST-29

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092220.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
 TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown9.69	9.690	2.3	ng	58844	2	10.918	520871	20.0
2-Propylnonanoi...	10.424	4.3	ng	113212	2	10.918	520871	20.0
unknown10.63	10.630	5.1	ng	133339	2	10.918	520871	20.0
unknown10.68	10.683	2.3	ng	59010	2	10.918	520871	20.0
unknown10.74	10.742	6.3	ng	164054	2	10.918	520871	20.0
unknown11.08	11.088	2.6	ng	69131	2	10.918	520871	20.0
unknown11.18	11.188	2.6	ng	68301	2	10.918	520871	20.0
unknown11.76	11.746	3.1	ng	81786	2	10.918	520871	20.0
unknown11.87	11.870	2.3	ng	60123	2	10.918	520871	20.0
unknown11.92	11.922	2.6	ng	67567	2	10.918	520871	20.0
n-Hexadecanoic ...	18.350	3.9	ng	193971	4	17.469	990005	20.0
Heptafluorobuty...	21.388	2.1	ng	132014	5	21.740	1265230	20.0