

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112922\
 Data File : BG055828.D
 Acq On : 29 Nov 2022 14:37
 Operator : CG/JU
 Sample : N5787-01
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SB-24-STOCK

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: BG055828.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.276	331	338	350	rBV	496640	769671	25.37%	5.261%
2	5.758	413	420	432	rBV	763656	1225390	40.39%	8.376%
3	6.375	519	525	532	rBV	29529	46614	1.54%	0.319%
4	7.373	686	695	710	rBV	716128	1297054	42.75%	8.866%
5	8.225	832	840	847	rBV	136263	234019	7.71%	1.600%
6	9.395	1031	1039	1050	rBV	442184	804104	26.50%	5.496%
7	10.799	1271	1278	1296	rBV	52387	143571	4.73%	0.981%
8	11.052	1314	1321	1328	rBV	189886	331141	10.91%	2.263%
9	13.472	1725	1733	1745	rVB	1224690	1861808	61.37%	12.726%
10	13.719	1769	1775	1783	rBV	24029	39302	1.30%	0.269%
11	14.847	1959	1967	1974	rBV	315743	485247	15.99%	3.317%
12	16.334	2213	2220	2235	rBV	1034326	1662967	54.81%	11.367%
13	17.585	2426	2433	2439	rBV	421488	645225	21.27%	4.410%
14	18.220	2536	2541	2545	rVB	27151	34918	1.15%	0.239%
15	18.443	2575	2579	2585	rBV2	76650	128103	4.22%	0.876%
16	18.860	2644	2650	2654	rBV	31630	41400	1.36%	0.283%
17	19.377	2730	2738	2743	rBV2	50134	73945	2.44%	0.505%
18	19.506	2755	2760	2764	rBV3	25337	35556	1.17%	0.243%
19	19.624	2775	2780	2786	rVB	56970	90712	2.99%	0.620%
20	19.706	2790	2794	2804	rVV3	36138	61748	2.04%	0.422%
21	19.988	2838	2842	2848	rVB	51504	75886	2.50%	0.519%
22	20.176	2867	2874	2879	rBV	2224944	3033923	100.00%	20.737%
23	21.874	3156	3163	3169	rBV2	428001	759861	25.05%	5.194%
24	25.264	3731	3740	3753	rVB2	265001	748134	24.66%	5.114%

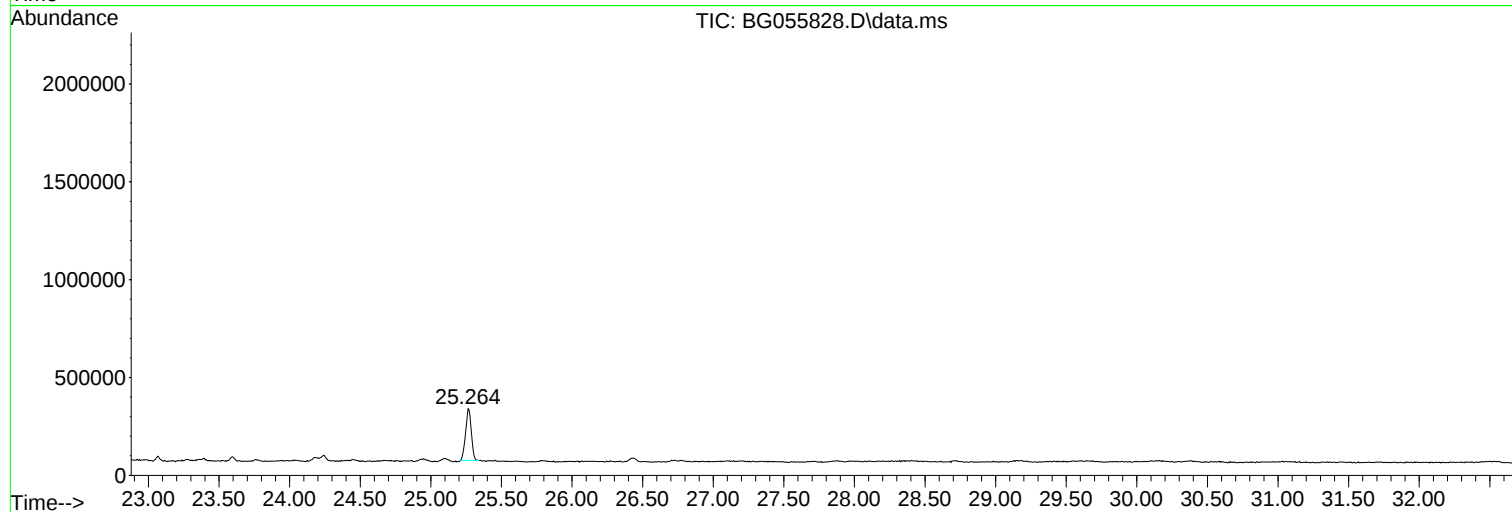
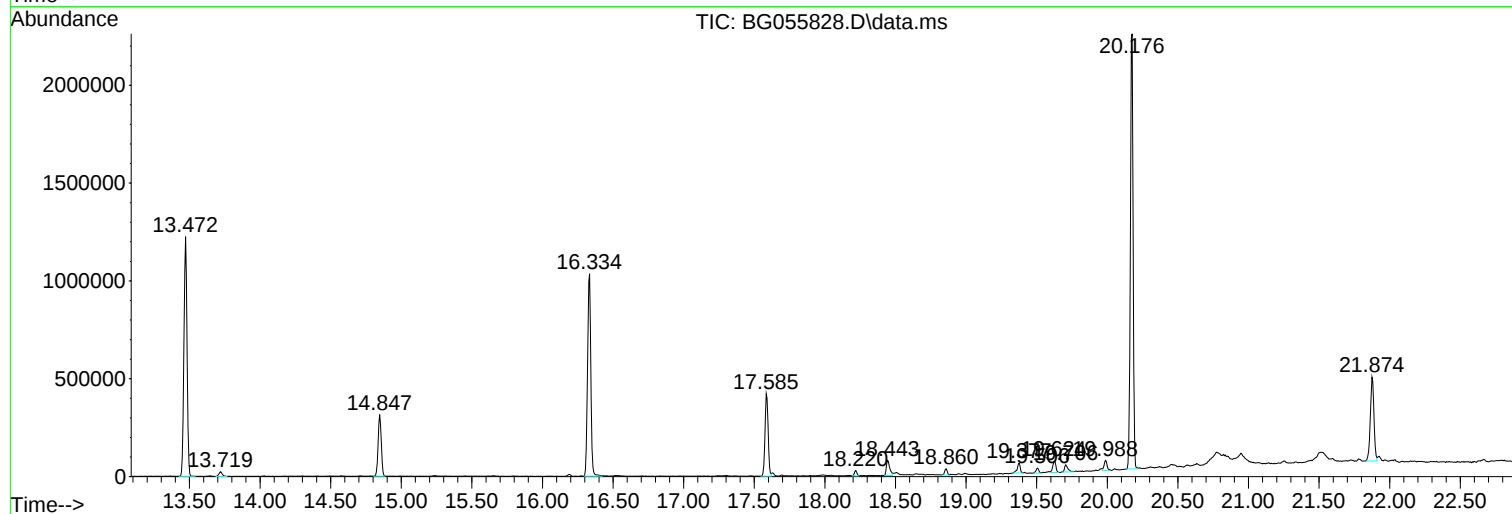
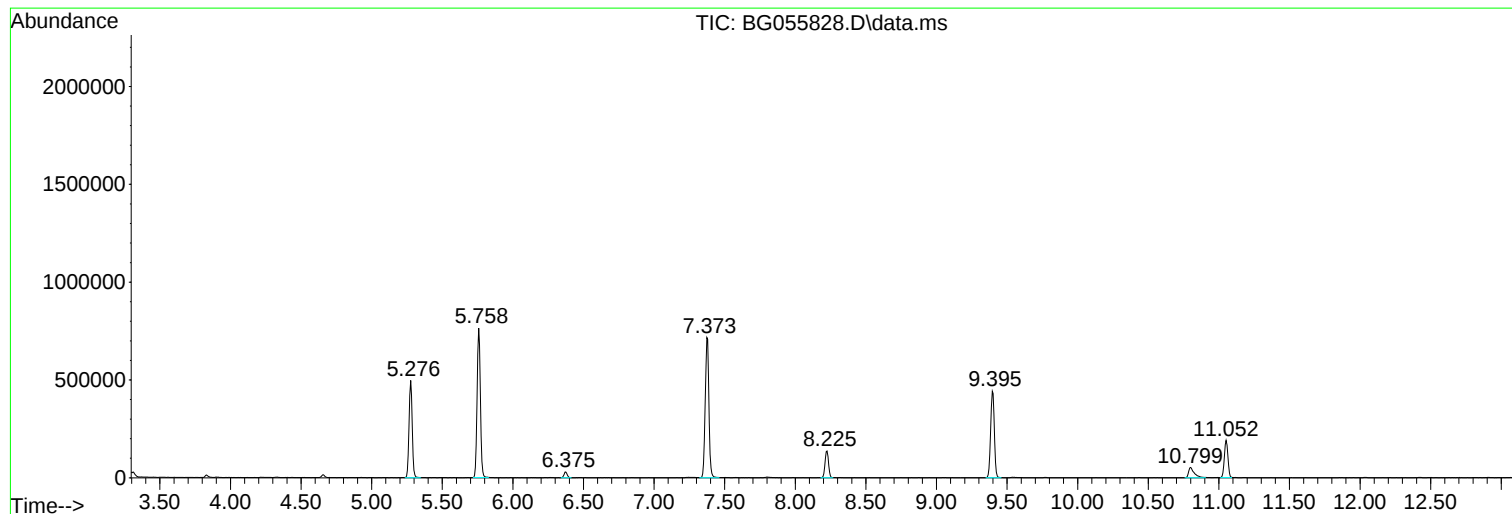
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Instrument :
BNA_G
ClientSampleId :
SB-24-STOCK

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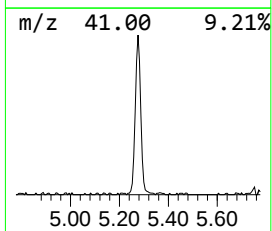
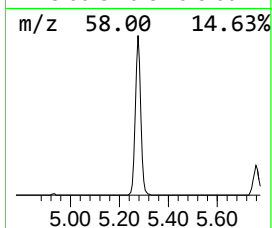
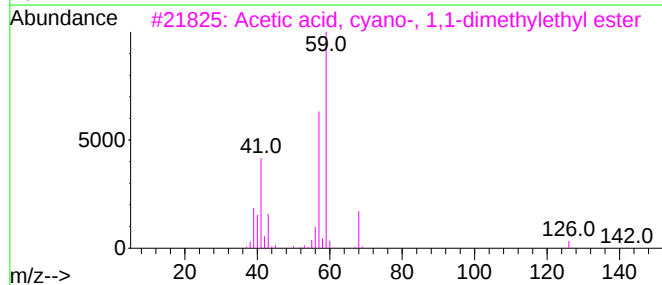
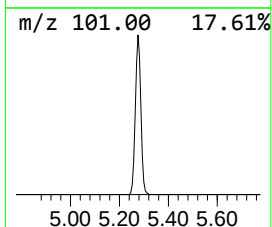
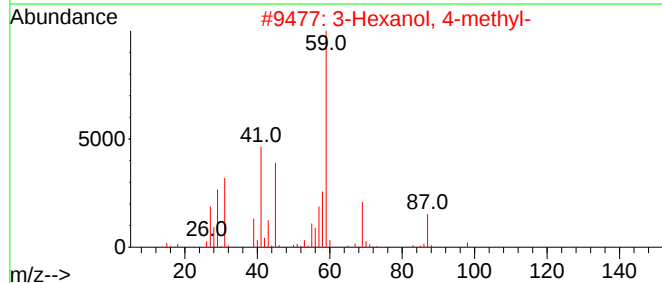
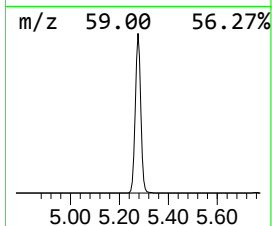
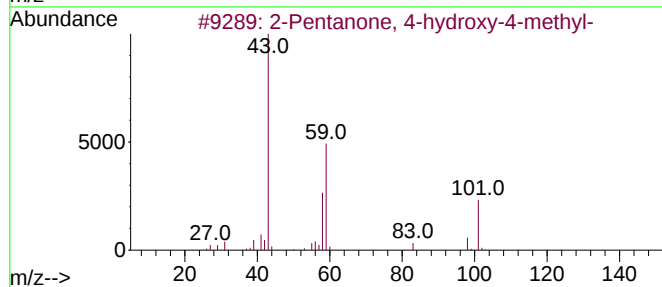
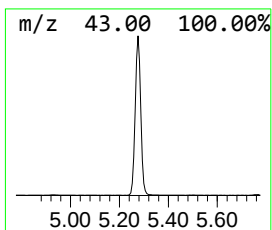
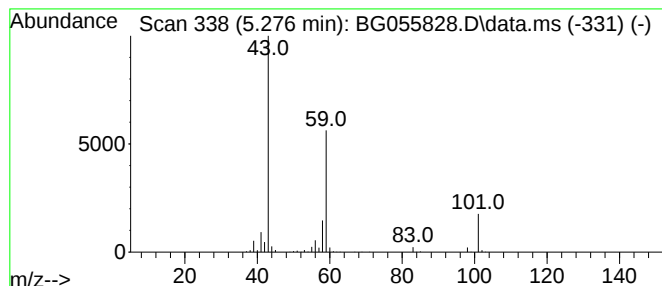
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG11622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.276	65.78 ng	769671	1,4-Dichlorobenzene-d4	8.225

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25		
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12		
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9		



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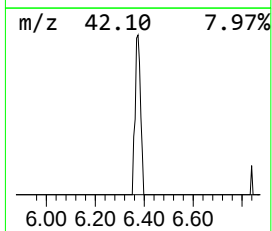
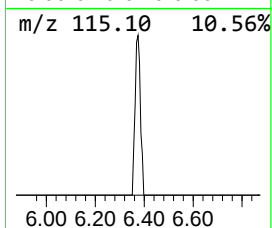
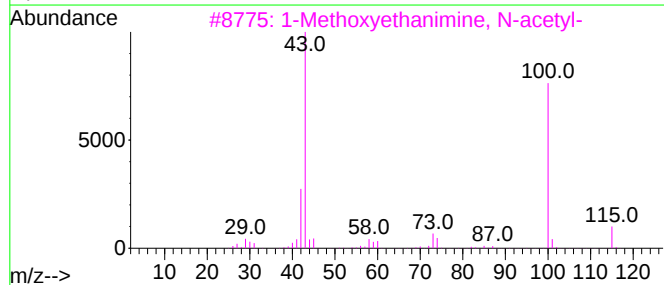
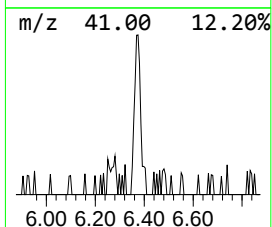
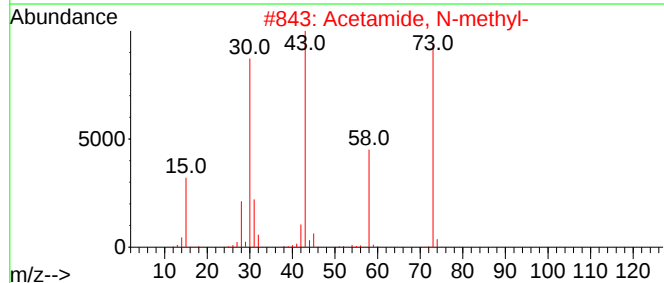
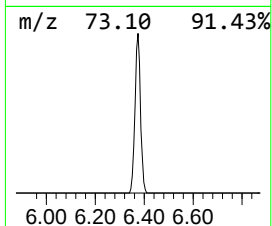
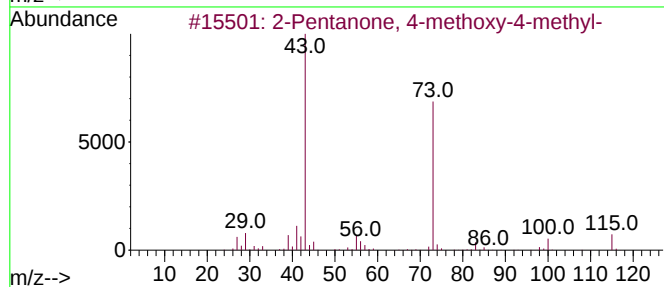
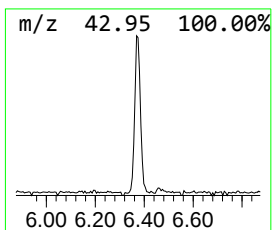
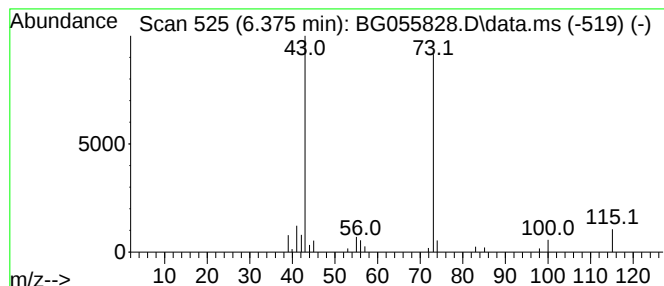
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.375	3.98 ng	46614	1,4-Dichlorobenzene-d4	8.225

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2		Acetamide, N-methyl-	73	C3H7NO	000079-16-3	43
3		1-Methoxyethanimine, N-acetyl-	115	C5H9NO2	099028-43-0	37
4		2-Propyn-1-ol, acetate	98	C5H6O2	000627-09-8	9
5		Hexane, 2-methyl-	100	C7H16	000591-76-4	9



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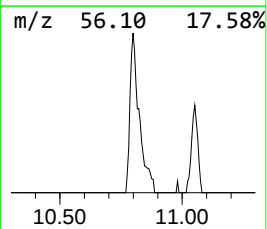
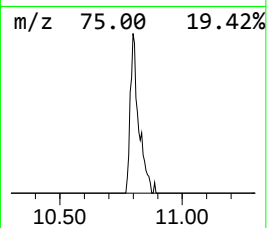
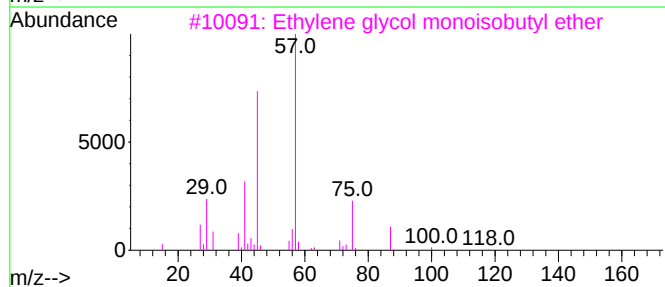
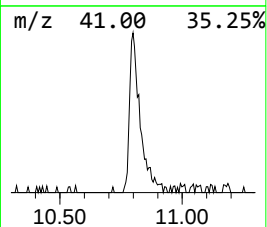
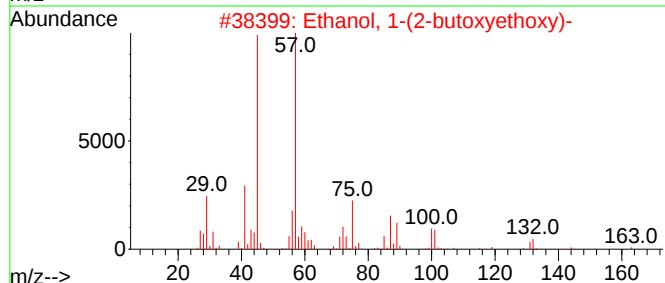
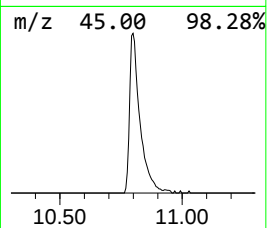
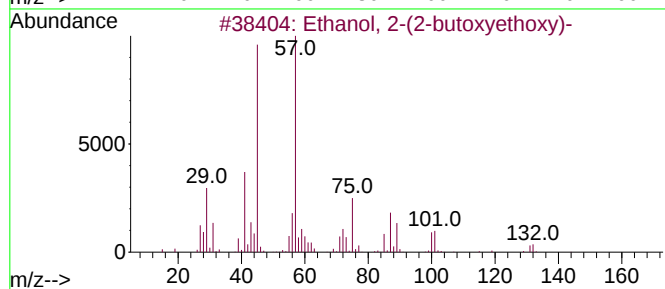
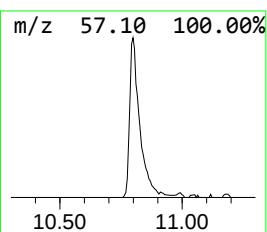
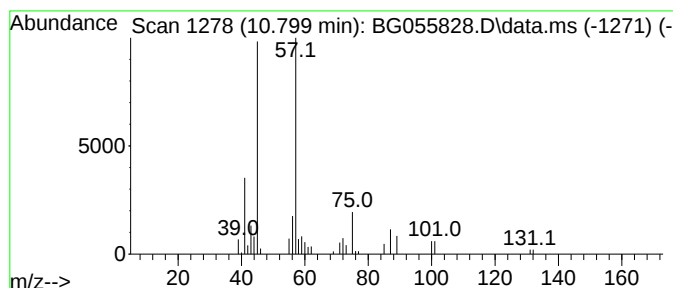
Instrument :
BNA_G
ClientSampleId :
SB-24-STOCK

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.799	8.67 ng	143571	Naphthalene-d8	11.052	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	72
4	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
5	Di-sec-Butyl ether	130	C8H18O	006863-58-7	50



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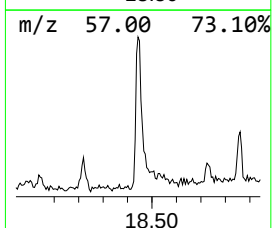
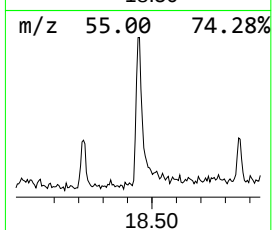
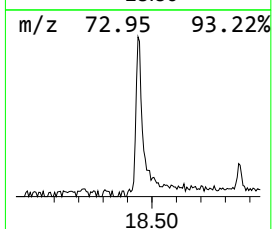
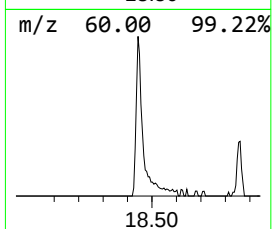
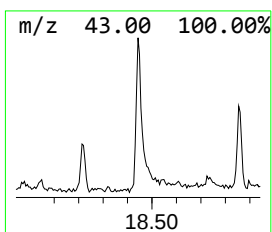
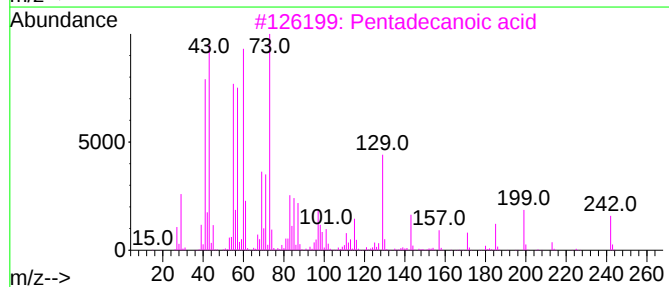
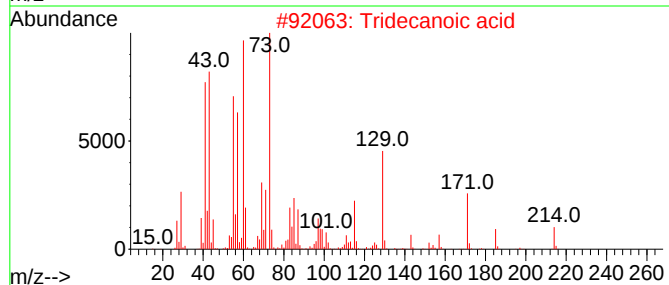
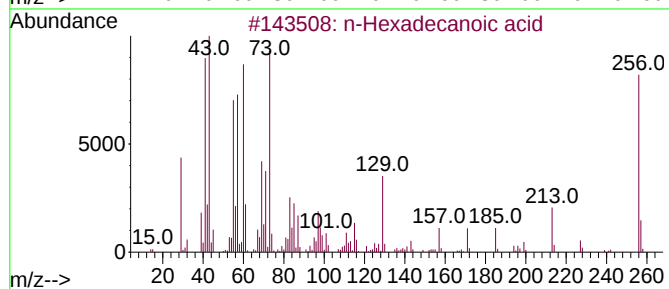
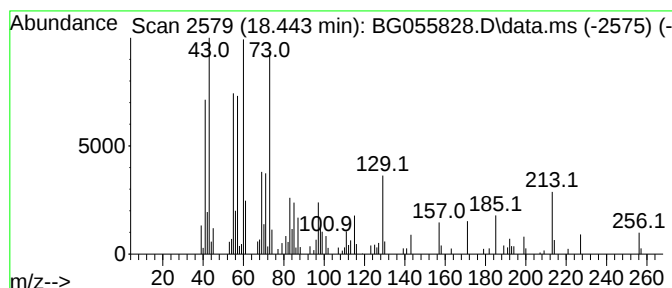
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.443	3.97 ng	128103	Phenanthrene-d10	17.585

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tridecanoic acid	214	C13H26O2	000638-53-9	95
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	68
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5			Nonanoic acid	158	C9H18O2	000112-05-0	49



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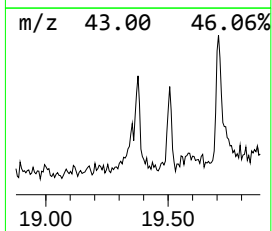
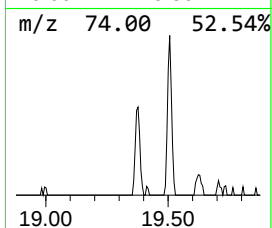
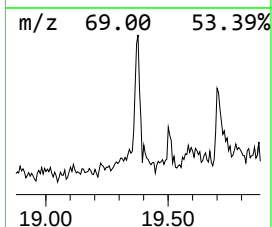
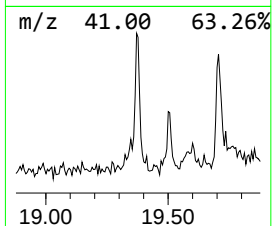
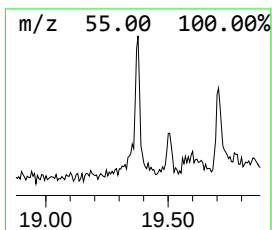
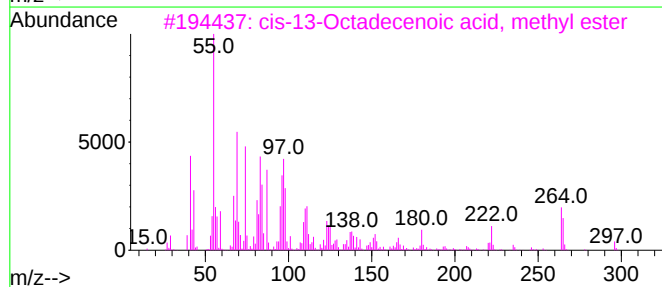
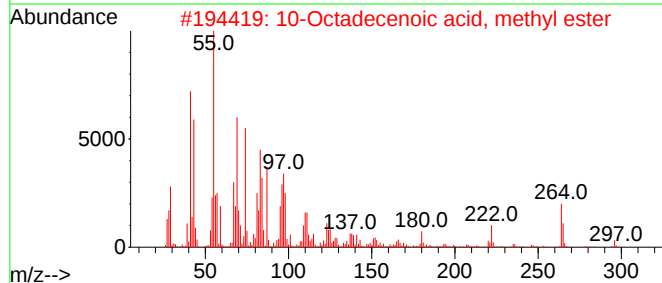
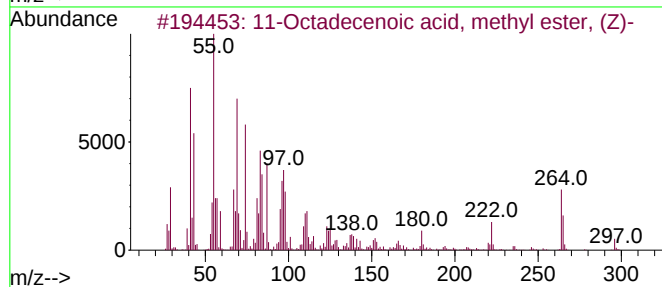
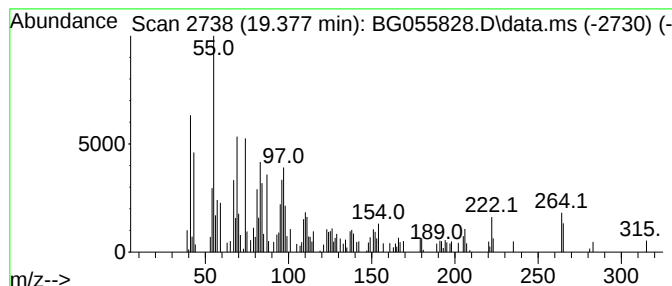
Instrument :
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ClientSampleId :
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 11-Octadecenoic acid, methy... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.377	2.29 ng	73945	Phenanthrene-d10	17.585	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11-Octadecenoic acid, methyl est...	296	C19H36O2	001937-63-9	94
2	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	94
3	cis-13-Octadecenoic acid, methyl...	296	C19H36O2	1010333-58-3	93
4	11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	91
5	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.276	65.8	ng	769671	1	8.225	234019	20.0
2-Pentanone, 4-...	6.375	4.0	ng	46614	1	8.225	234019	20.0
Ethanol, 2-(2-b...	10.799	8.7	ng	143571	2	11.052	331141	20.0
n-Hexadecanoic ...	18.443	4.0	ng	128103	4	17.585	645225	20.0
11-Octadecenoic...	19.377	2.3	ng	73945	4	17.585	645225	20.0