

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081022\
 Data File : BM036192.D
 Acq On : 10 Aug 2022 15:02
 Operator : CG/JU
 Sample : N3971-07
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 MW-12

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_M\Methods\8270-BM080122.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM036192.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.281	198	203	216	rBV	1339434	1840452	13.88%	2.896%
2	4.928	305	313	321	rBV	319746	498931	3.76%	0.785%
3	5.416	390	396	411	rVB	2292864	3247218	24.50%	5.110%
4	6.475	570	576	588	rBV	341662	491434	3.71%	0.773%
5	7.034	664	671	682	rBV	1344626	2083060	15.71%	3.278%
6	7.834	799	807	813	rBV	911780	1409338	10.63%	2.218%
7	7.904	813	819	832	rVV	250341	441643	3.33%	0.695%
8	8.457	906	913	924	rBV	106310	189273	1.43%	0.298%
9	9.004	999	1006	1016	rBV	2662494	4245502	32.03%	6.681%
10	9.151	1026	1031	1042	rVB4	63919	136206	1.03%	0.214%
11	9.569	1095	1102	1111	rVB	146640	246684	1.86%	0.388%
12	9.992	1168	1174	1181	rVB	124770	211040	1.59%	0.332%
13	10.428	1241	1248	1257	rBV3	70560	141030	1.06%	0.222%
14	10.639	1276	1284	1291	rBV	1160427	1959913	14.79%	3.084%
15	11.469	1418	1425	1433	rBV2	106501	188132	1.42%	0.296%
16	11.604	1443	1448	1460	rVB	158503	343307	2.59%	0.540%
17	13.104	1695	1703	1717	rBV	6621040	9455921	71.34%	14.880%
18	13.333	1736	1742	1748	rBV	2393882	3299438	24.89%	5.192%
19	14.474	1930	1936	1944	rVB	1692760	2420170	18.26%	3.808%
20	15.298	2067	2076	2083	rVB	80710	149488	1.13%	0.235%
21	15.833	2162	2167	2172	rBV	112934	159676	1.20%	0.251%
22	15.968	2183	2190	2206	rBV	5003947	7083667	53.44%	11.147%
23	17.215	2396	2402	2411	rBV	1890572	2687279	20.27%	4.229%
24	17.886	2512	2516	2521	rVB	214214	260952	1.97%	0.411%
25	18.115	2550	2555	2564	rBV	296236	504450	3.81%	0.794%
26	19.398	2769	2773	2780	rBV	128349	206882	1.56%	0.326%
27	19.845	2843	2849	2854	rBV	10922240	13255331	100.00%	20.859%
28	21.397	3108	3113	3118	rBV	2547867	3130199	23.61%	4.926%
29	23.744	3506	3512	3521	rVB2	1675535	3261631	24.61%	5.133%

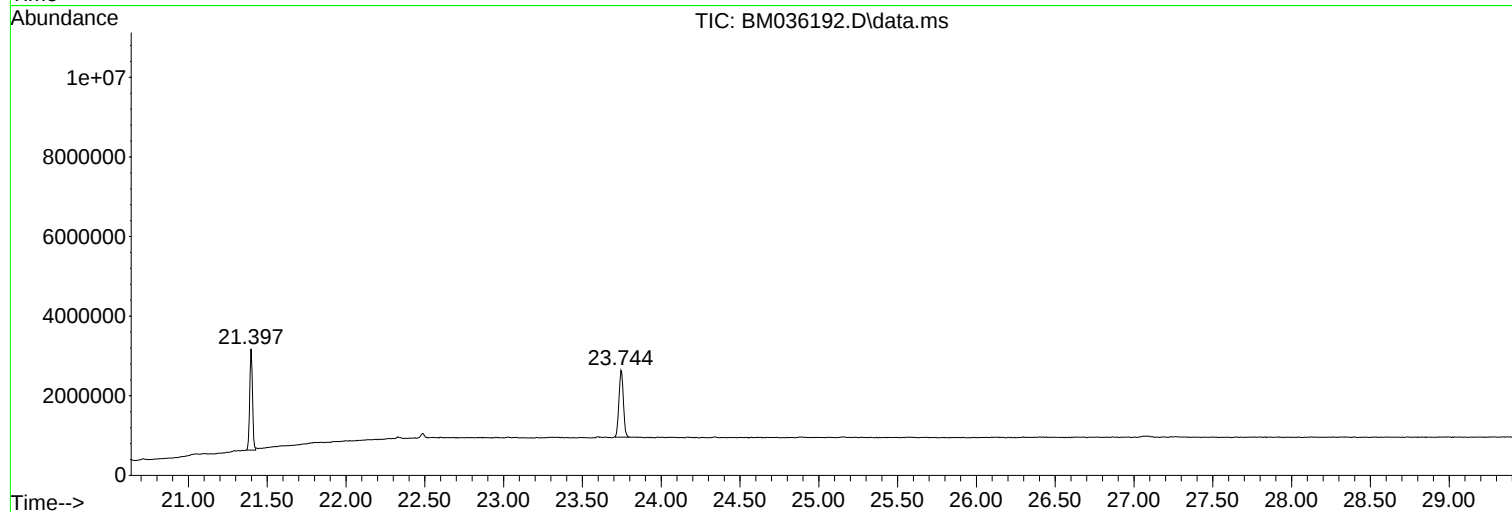
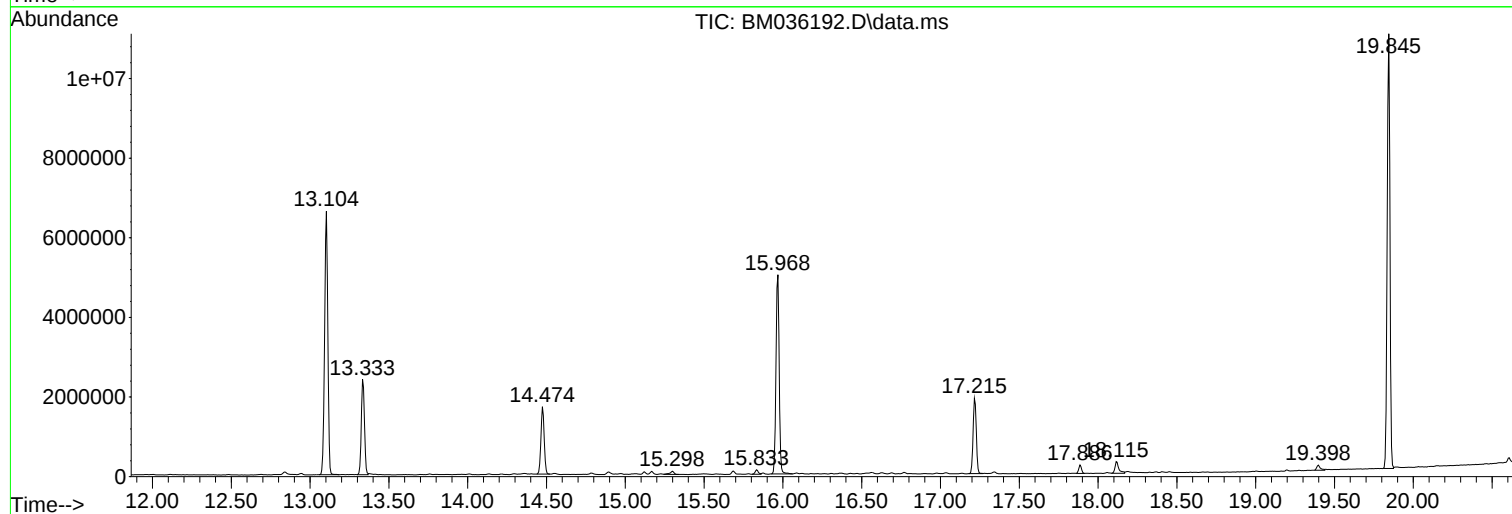
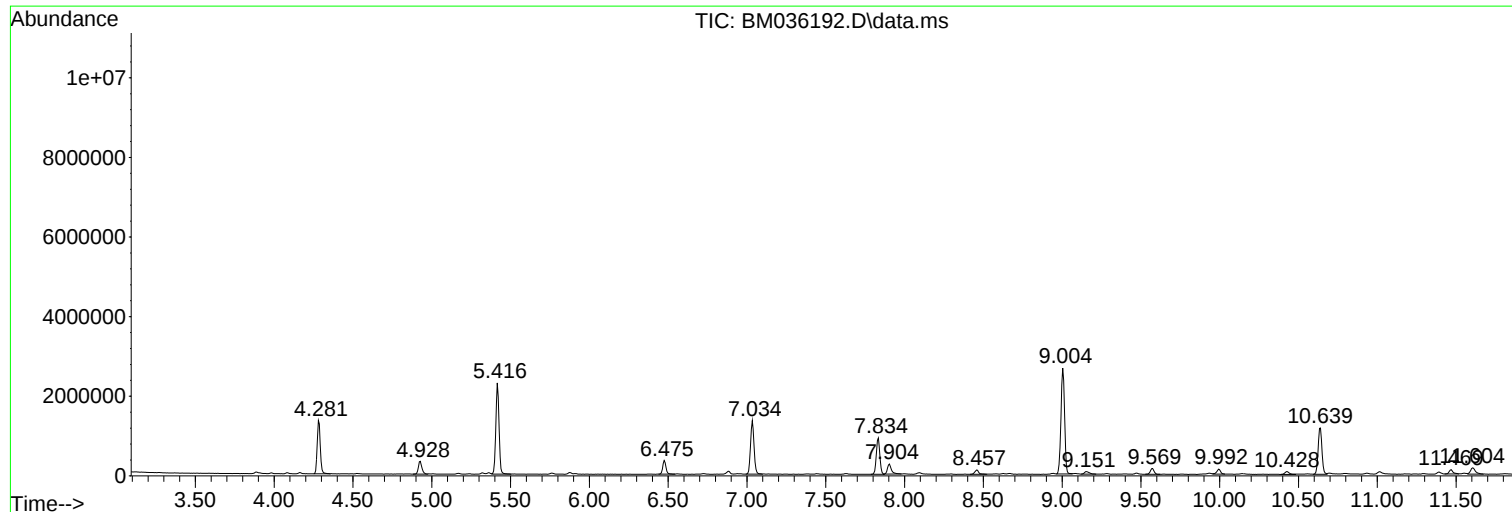
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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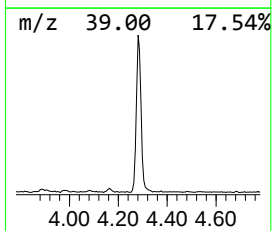
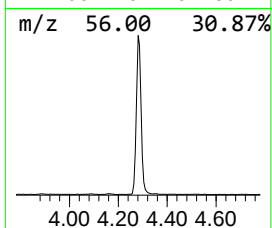
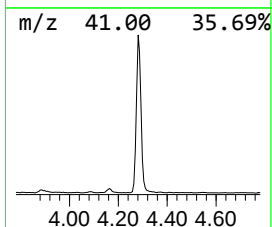
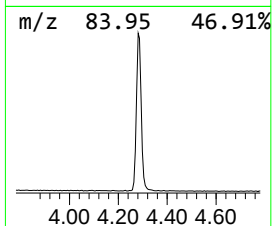
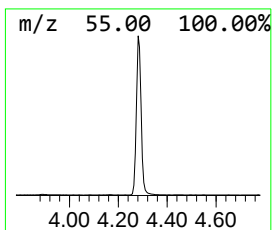
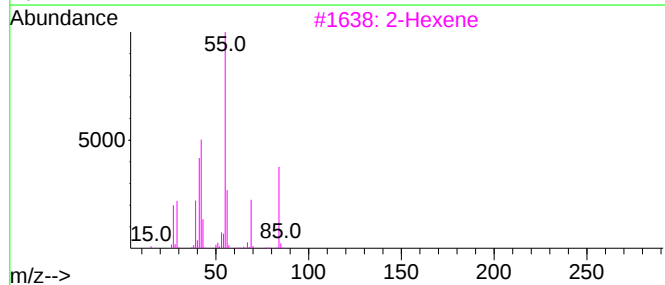
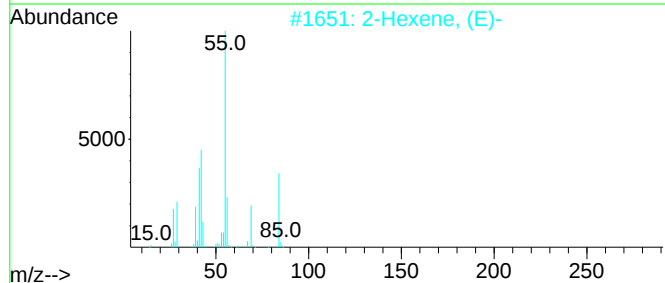
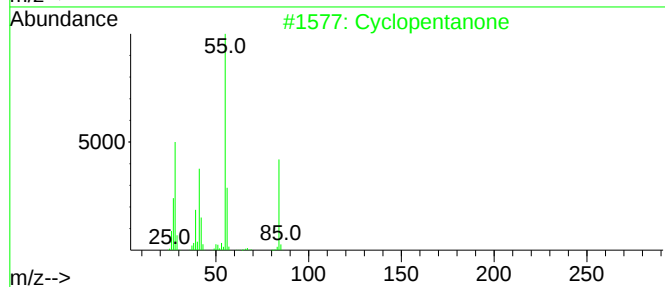
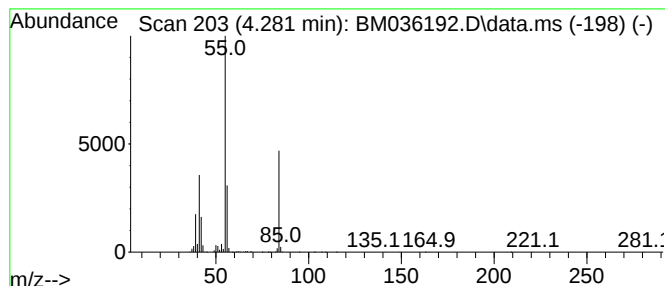
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Cyclopentanone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD			R.T.
4.281	26.12 ng	1840450	1,4-Dichlorobenzene-d4			7.834
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Cyclopentanone		84	C5H8O	000120-92-3	91
2	2-Hexene, (E)-		84	C6H12	004050-45-7	64
3	2-Hexene		84	C6H12	000592-43-8	59
4	3-Hexene, (Z)-		84	C6H12	007642-09-3	59
5	2H-Pyran, 3,4-dihydro-		84	C5H8O	000110-87-2	45



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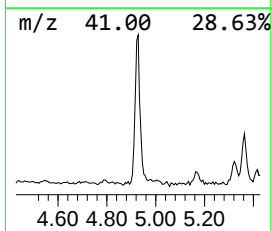
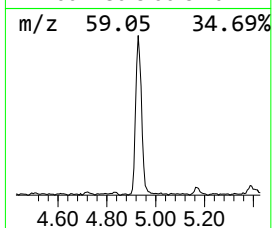
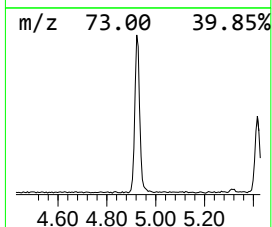
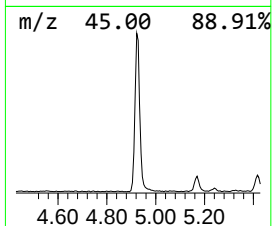
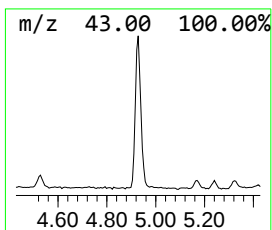
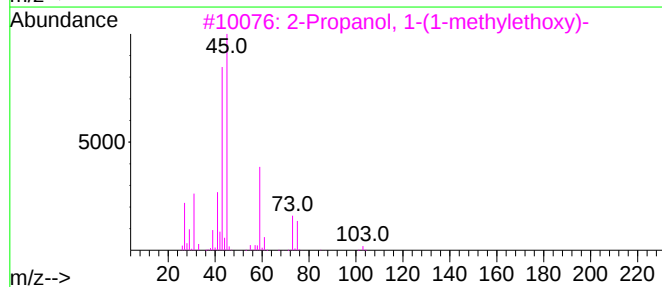
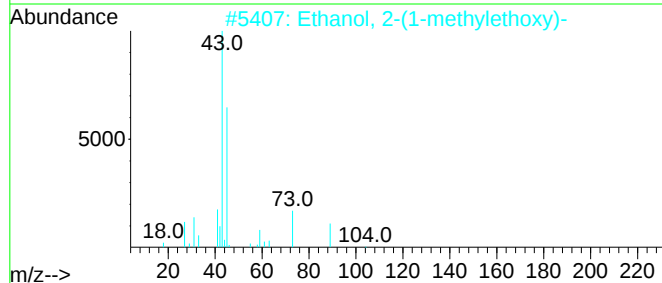
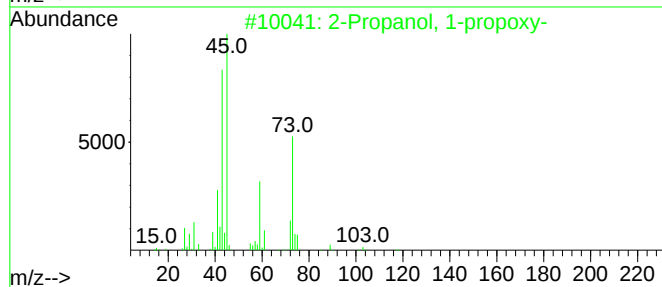
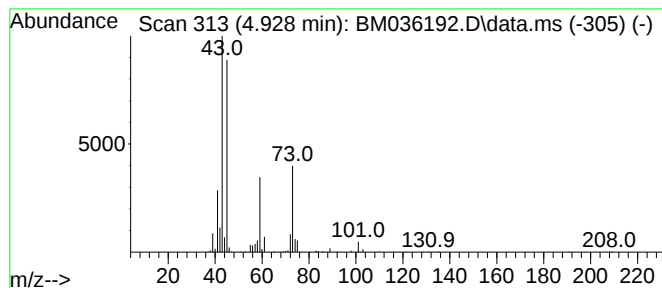
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TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Propanol, 1-propoxy- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.928	7.08 ng	498931	1,4-Dichlorobenzene-d4	7.834

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Propanol, 1-propoxy-	118	C6H14O2	001569-01-3	78
2		Ethanol, 2-(1-methylethoxy)-	104	C5H12O2	000109-59-1	72
3		2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	72
4		Sulfurous acid, bis(1-methylethy...	166	C6H14O3S	004773-13-1	50
5		Butane, 1-(1-methylethoxy)-	116	C7H16O	001860-27-1	50



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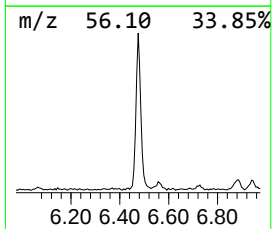
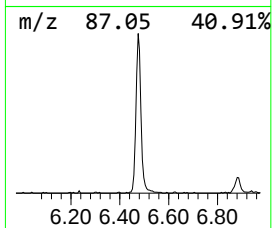
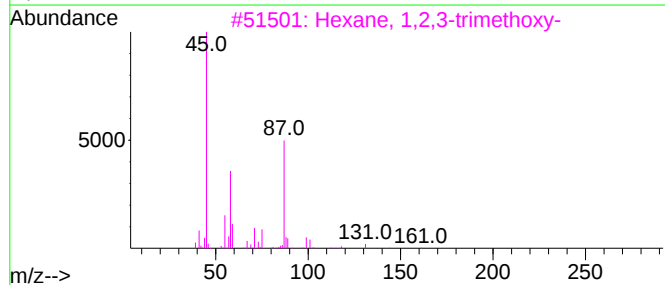
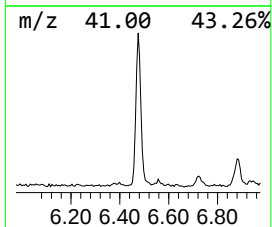
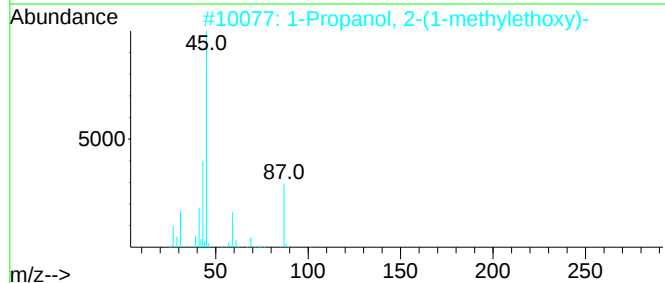
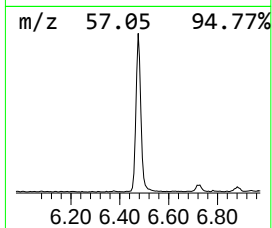
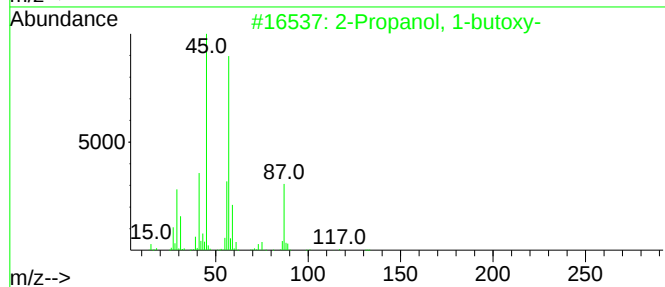
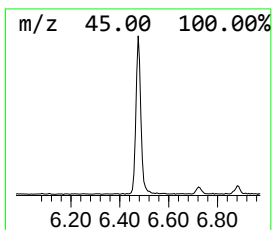
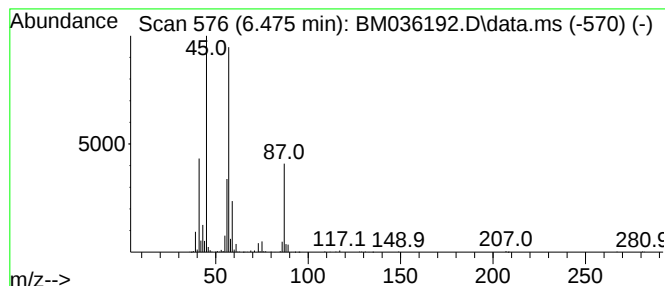
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Propanol, 1-butoxy- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.475	6.97 ng	491434	1,4-Dichlorobenzene-d4	7.834

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-butoxy-			132	C7H16O2	005131-66-8	90
2	1-Propanol, 2-(1-methylethoxy)-			118	C6H14O2	003944-37-4	53
3	Hexane, 1,2,3-trimethoxy-			176	C9H20O3	020637-29-0	50
4	Propane, 1,1'-[ethylidenebis(oxy...]			146	C8H18O2	000105-82-8	50
5	Formic acid, 1-methylpropyl ester			102	C5H10O2	000589-40-2	50



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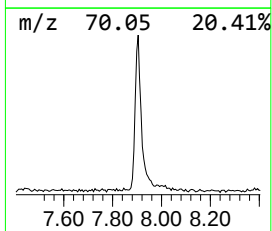
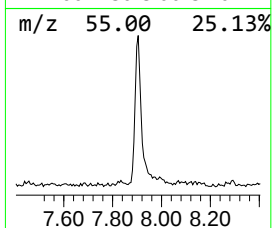
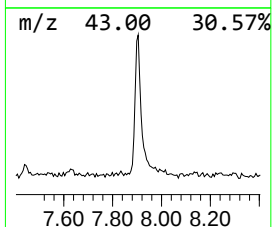
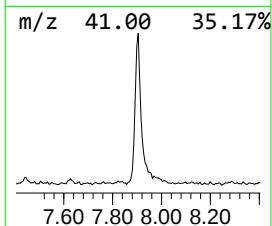
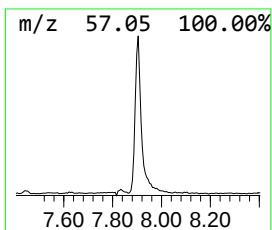
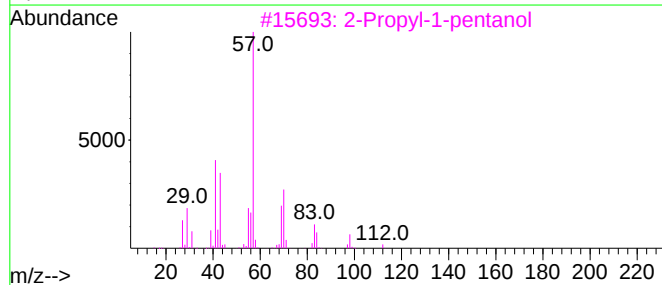
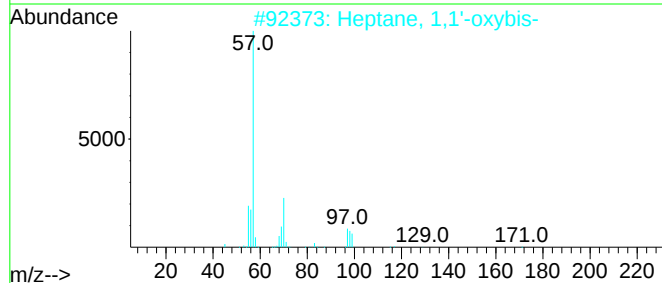
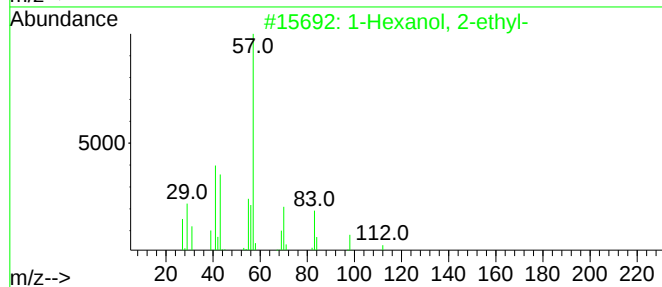
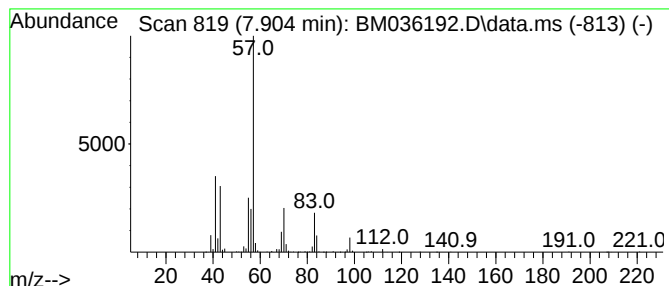
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Peak Number 4 1-Hexanol, 2-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.904	6.27 ng	441643	1,4-Dichlorobenzene-d4	7.834

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2		Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	64
3		2-Propyl-1-pentanol	130	C8H18O	058175-57-8	53
4		2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	53
5		Oxalic acid, isobutyl octyl ester	258	C14H26O4	1000309-37-3	50



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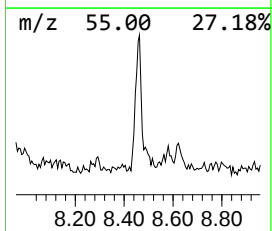
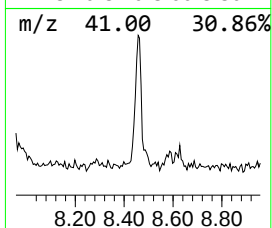
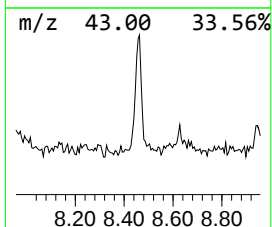
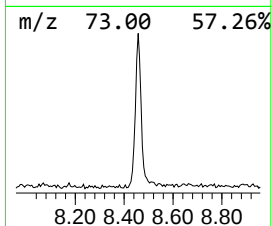
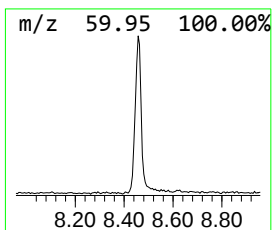
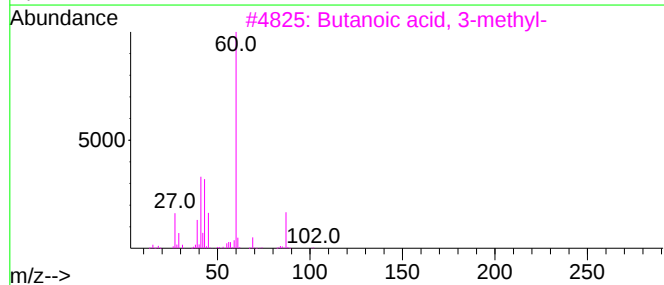
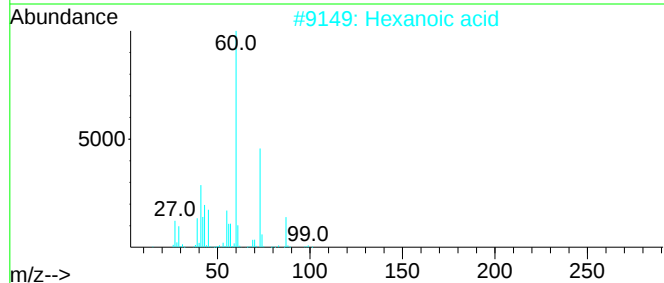
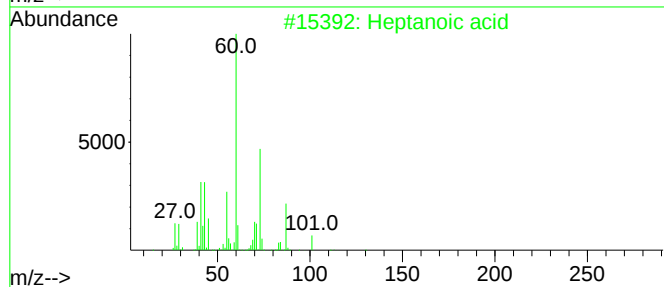
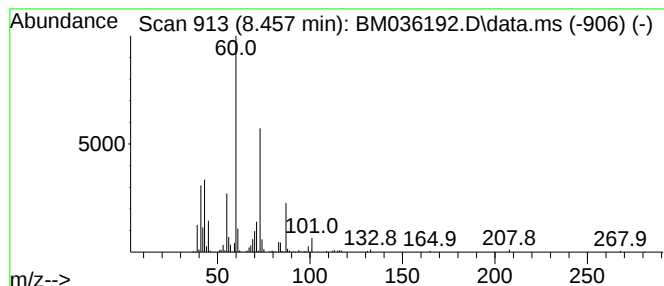
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Peak Number 5 Heptanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.457	2.69 ng	189273	1,4-Dichlorobenzene-d4	7.834

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptanoic acid	130	C7H14O2	000111-14-8	86
2			Hexanoic acid	116	C6H12O2	000142-62-1	64
3			Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	59
4			Pentanoic acid	102	C5H10O2	000109-52-4	50
5			Pentanoic acid, 3-methyl-	116	C6H12O2	000105-43-1	45



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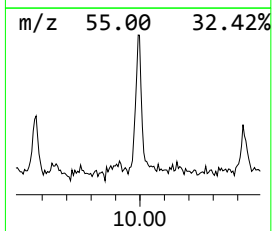
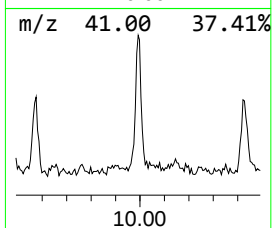
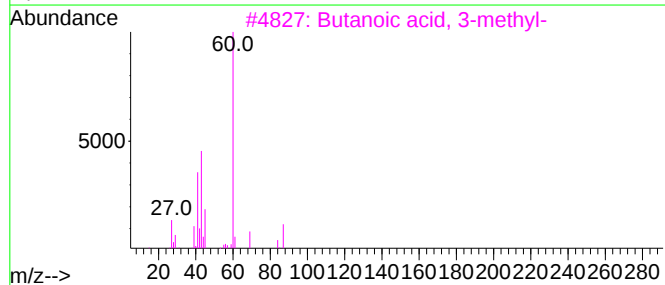
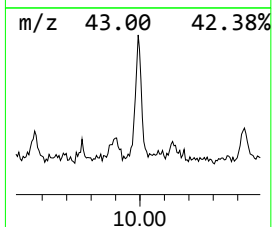
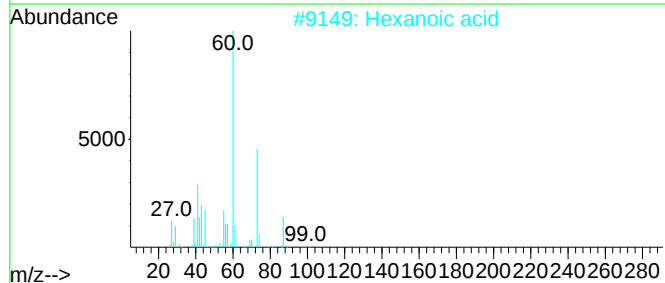
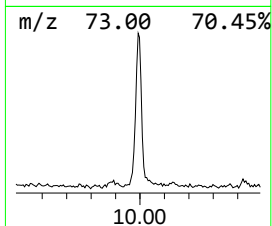
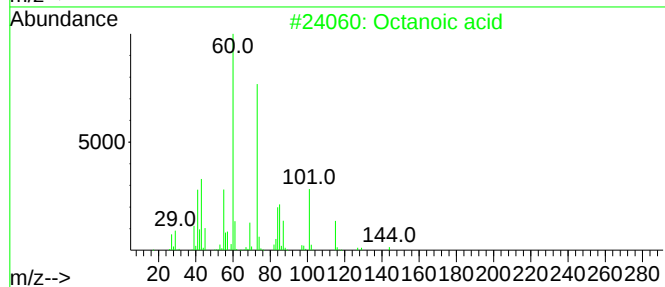
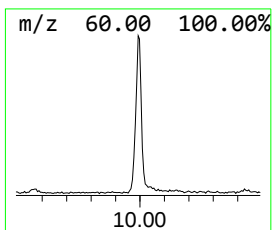
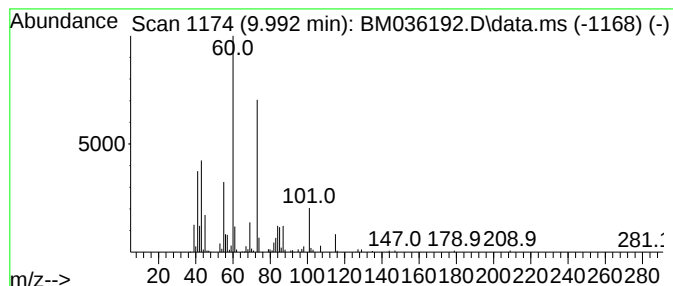
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.992	2.15 ng	211040	Naphthalene-d8	10.639

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octanoic acid	144	C8H16O2	000124-07-2	91
2			Hexanoic acid	116	C6H12O2	000142-62-1	64
3			Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	59
4			Nonanoic acid	158	C9H18O2	000112-05-0	53
5			Pentanoic acid	102	C5H10O2	000109-52-4	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081022\
Data File : BM036192.D
Acq On : 10 Aug 2022 15:02
Operator : CG/JU
Sample : N3971-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

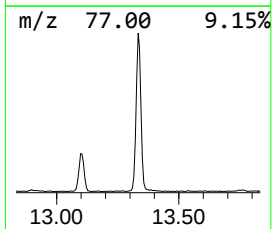
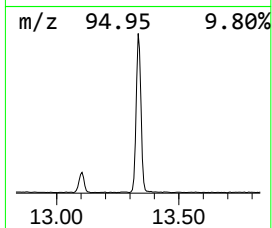
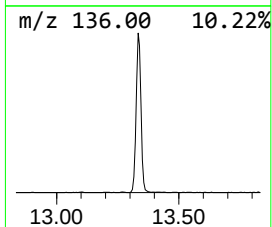
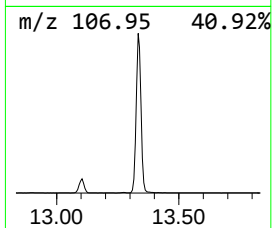
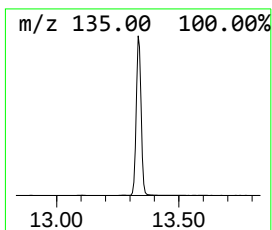
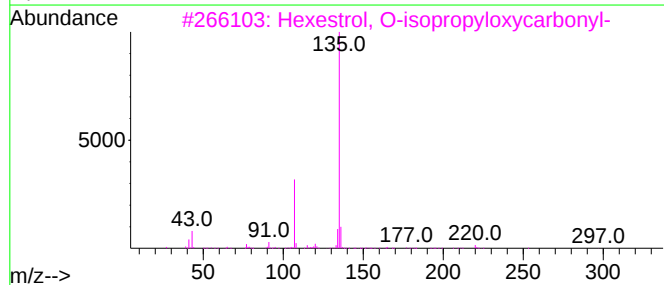
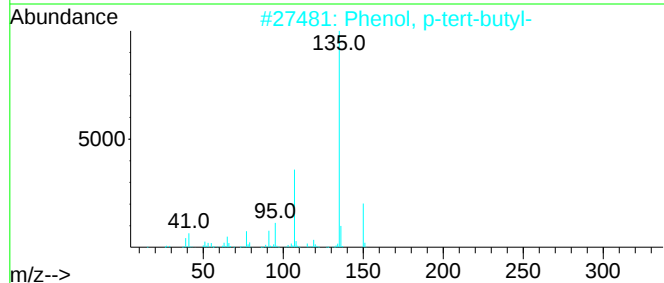
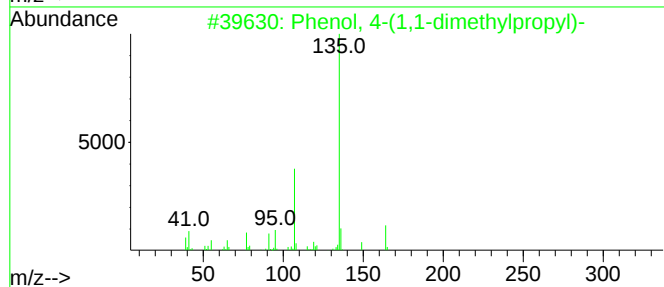
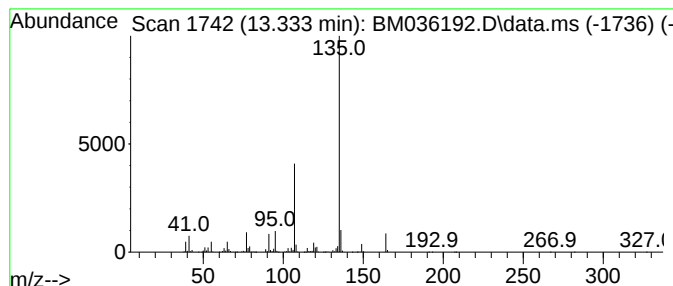
Instrument :
BNA_M
ClientSampleId :
MW-12

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Phenol, 4-(1,1-dimethylprop... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.333	27.27 ng	3299440	Acenaphthene-d10		14.474	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Phenol, 4-(1,1-dimethylpropyl)-		164	C11H16O	000080-46-6	94
2	Phenol, p-tert-butyl-		150	C10H14O	000098-54-4	90
3	Hexestrol, O-isopropylloxycarbonyl-		356	C22H28O4	1000487-68-4	64
4	Imidazo[1,2-c]pyrimidin-5-ol		135	C6H5N3O	055662-66-3	64
5	4,6-Bis(4-ethoxybenzylthio)-5-ni...		457	C22H23N3O4S2	325957-76-4	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081022\
Data File : BM036192.D
Acq On : 10 Aug 2022 15:02
Operator : CG/JU
Sample : N3971-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MW-12

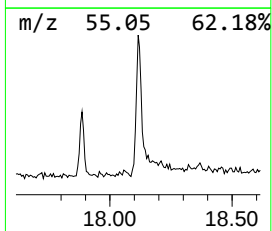
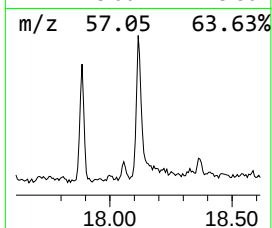
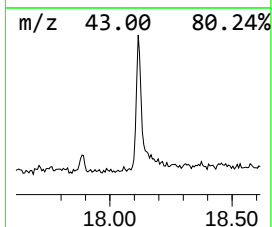
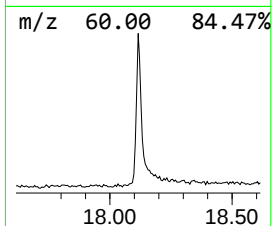
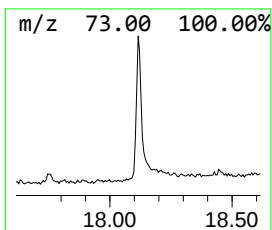
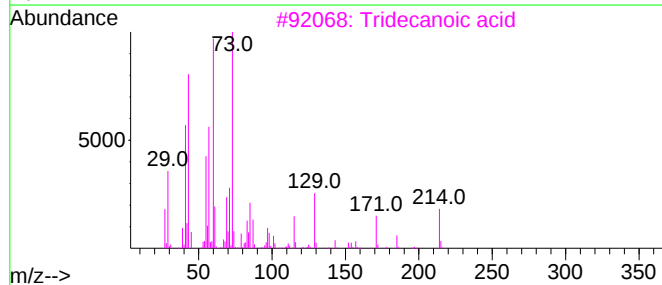
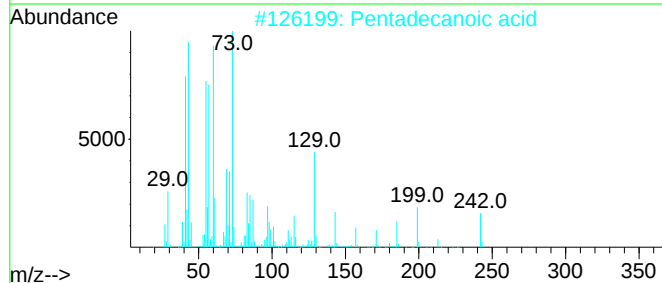
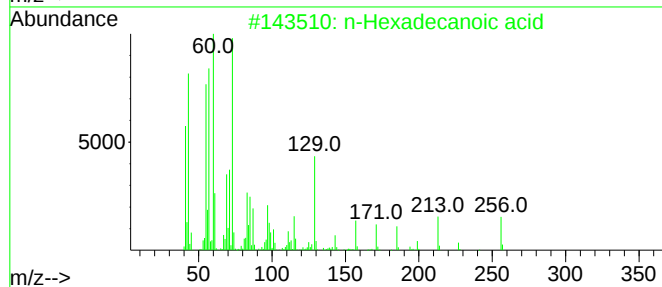
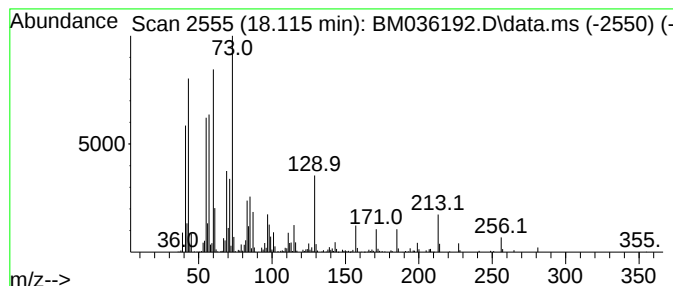
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.115	3.75 ng	504450	Phenanthrene-d10	17.215

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3			Tridecanoic acid	214	C13H26O2	000638-53-9	81
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	81
5			Dodecanoic acid	200	C12H24O2	000143-07-7	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081022\
Data File : BM036192.D
Acq On : 10 Aug 2022 15:02
Operator : CG/JU
Sample : N3971-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MW-12

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.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
Cyclopentanone	4.281	26.1	ng	1840450	1	7.834	1409340	20.0
2-Propanol, 1-p...	4.928	7.1	ng	498931	1	7.834	1409340	20.0
2-Propanol, 1-b...	6.475	7.0	ng	491434	1	7.834	1409340	20.0
1-Hexanol, 2-et...	7.904	6.3	ng	441643	1	7.834	1409340	20.0
Heptanoic acid	8.457	2.7	ng	189273	1	7.834	1409340	20.0
Octanoic acid	9.992	2.1	ng	211040	2	10.639	1959910	20.0
Phenol, 4-(1,1-...	13.333	27.3	ng	3299440	3	14.474	2420170	20.0
n-Hexadecanoic ...	18.115	3.8	ng	504450	4	17.215	2687280	20.0