

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP081524\
 Data File : BP021524.D
 Acq On : 15 Aug 2024 22:14
 Operator : RC/JU
 Sample : P3573-10
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 S-856-J-S0-4-4.5-080924

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_P\Methods\8270E-BP081324.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP021524.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.028	3	7	25	rVB	3818512	5024742	42.65%	6.371%
2	3.540	90	94	106	rVB	295892	402775	3.42%	0.511%
3	4.934	324	331	340	rVB	232651	332208	2.82%	0.421%
4	5.393	403	409	418	rVB	4855987	6924228	58.77%	8.779%
5	6.957	667	675	692	rVB	4621506	7132923	60.54%	9.044%
6	7.804	811	819	826	rBV	1350400	2238668	19.00%	2.838%
7	8.945	1004	1013	1021	rBV	2482407	4271634	36.25%	5.416%
8	9.504	1102	1108	1114	rVB	91505	138204	1.17%	0.175%
9	9.887	1164	1173	1179	rBV	73623	128847	1.09%	0.163%
10	10.587	1284	1292	1301	rBV	1697367	2946287	25.01%	3.736%
11	11.328	1412	1418	1426	rBV	287527	505574	4.29%	0.641%
12	11.398	1426	1430	1439	rVB	92738	159767	1.36%	0.203%
13	12.704	1642	1652	1661	rBV	117977	201432	1.71%	0.255%
14	13.057	1704	1712	1724	rBV	5323263	8323384	70.64%	10.553%
15	14.439	1940	1947	1954	rBV	2468478	3597142	30.53%	4.561%
16	14.657	1978	1984	1985	rBV2	92834	133704	1.13%	0.170%
17	14.775	1998	2004	2010	rVB	151734	209794	1.78%	0.266%
18	15.939	2195	2202	2212	rBV	4633119	6460546	54.83%	8.191%
19	17.227	2415	2421	2431	rVB	2988957	4327097	36.72%	5.486%
20	18.168	2573	2581	2591	rBV	555021	1034212	8.78%	1.311%
21	19.498	2802	2807	2820	rBV	275576	482206	4.09%	0.611%
22	19.751	2844	2850	2854	rBV2	109297	176678	1.50%	0.224%
23	19.945	2877	2883	2893	rVB	9679022	11782468	100.00%	14.939%
24	21.351	3117	3122	3131	rBV	460798	850155	7.22%	1.078%
25	21.668	3170	3176	3184	rBV2	3121913	5051155	42.87%	6.404%
26	22.633	3336	3340	3352	rVB2	109958	211319	1.79%	0.268%
27	23.892	3551	3554	3564	rVB4	101798	236796	2.01%	0.300%
28	25.080	3745	3756	3769	rVB	2148814	5587787	47.42%	7.085%

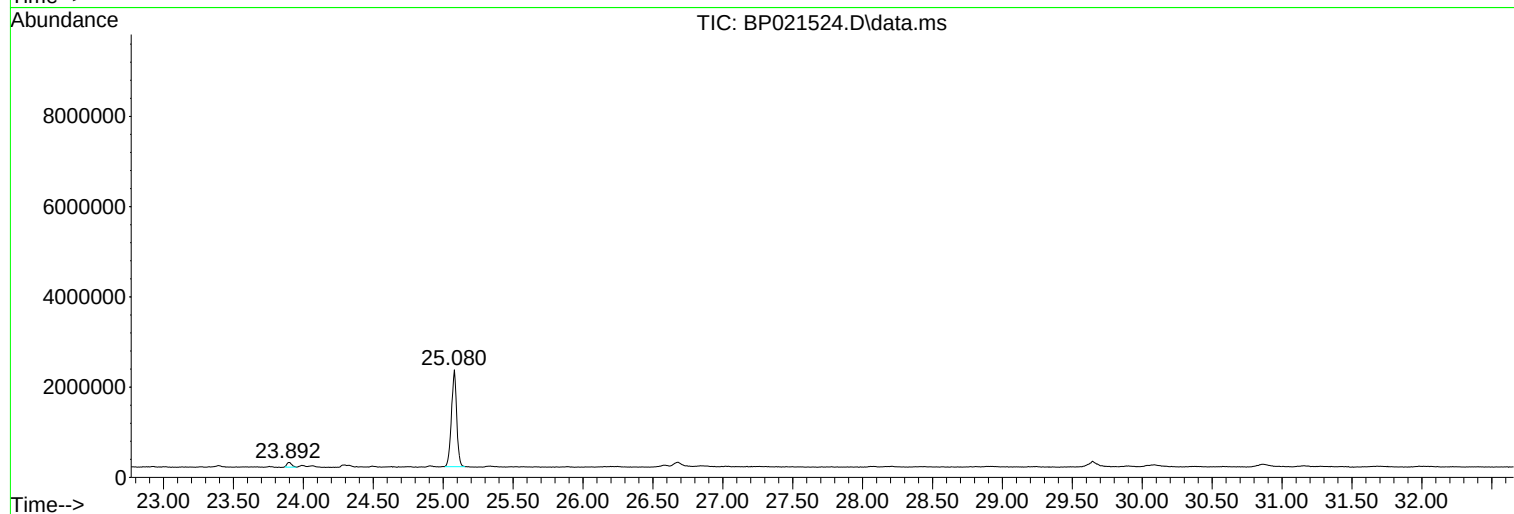
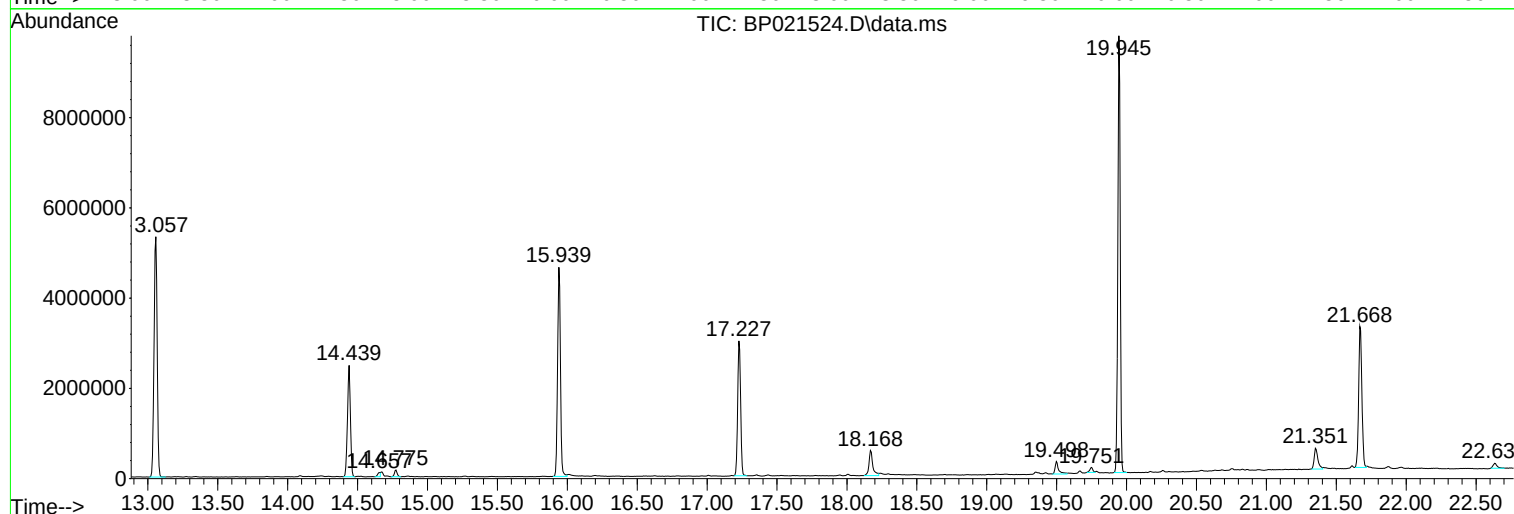
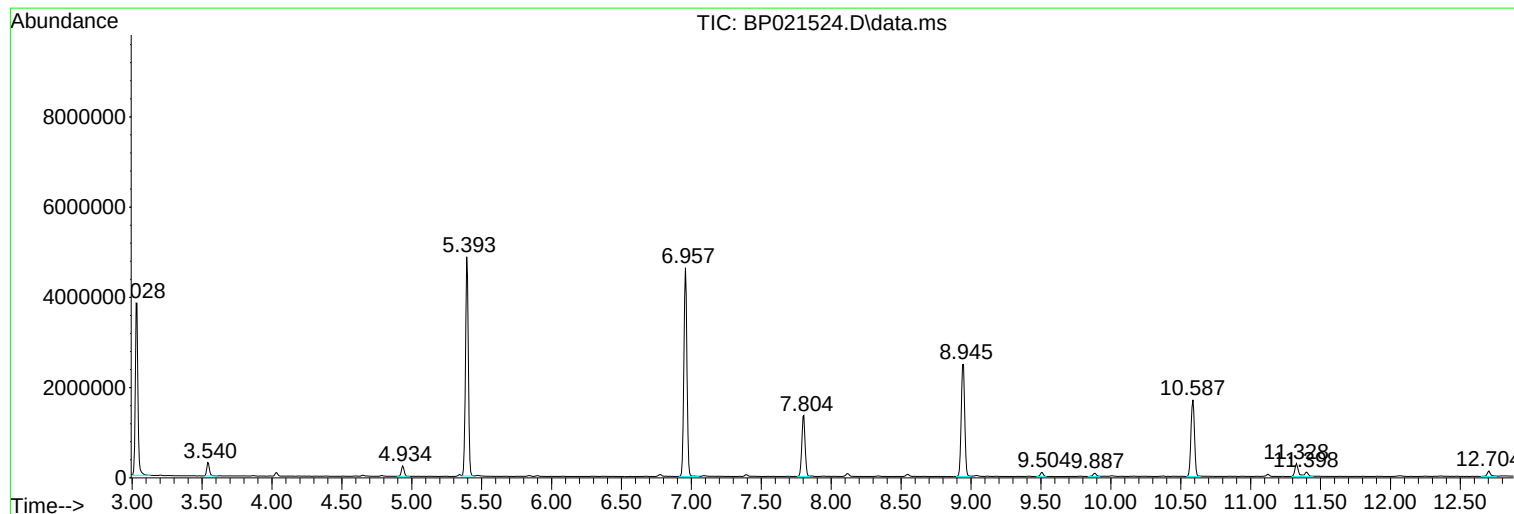
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP081324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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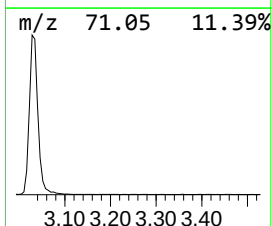
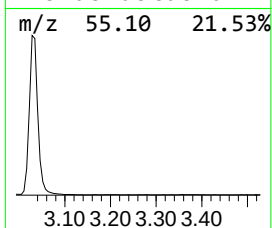
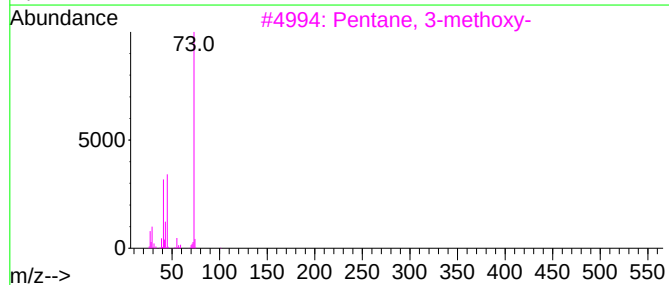
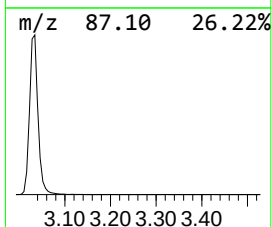
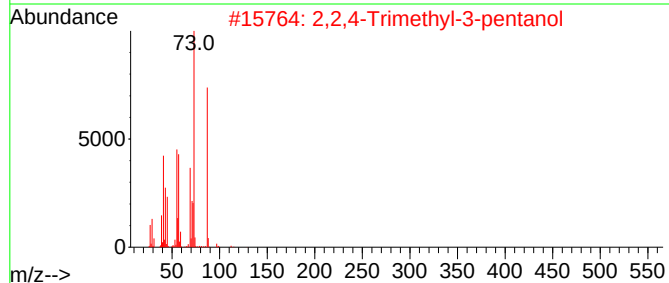
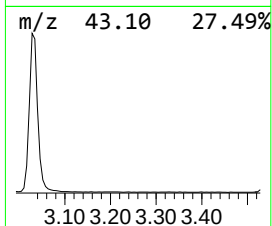
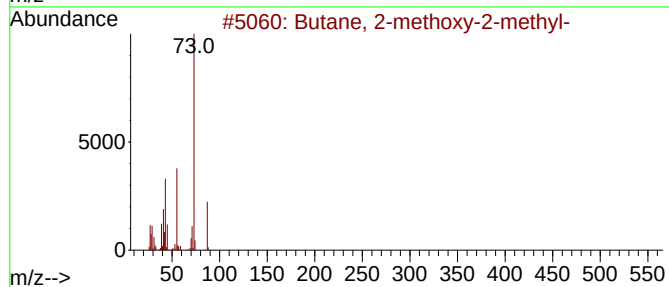
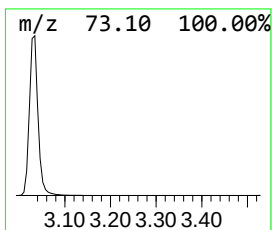
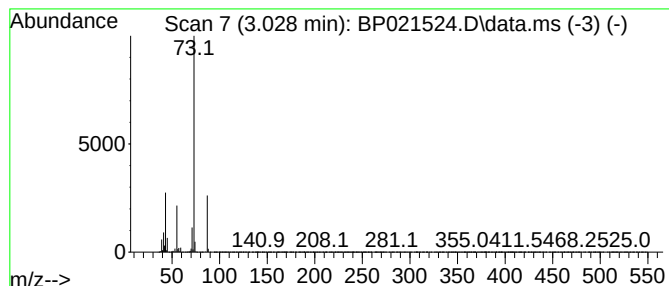
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.028	44.89 ng	5024740	1,4-Dichlorobenzene-d4	7.804

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	43
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
5			N-Ethylformamide	73	C3H7NO	000627-45-2	9



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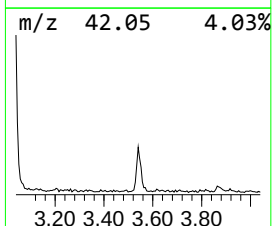
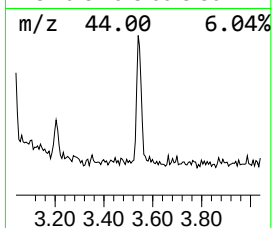
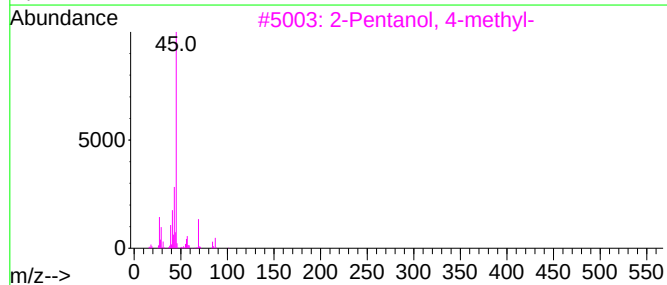
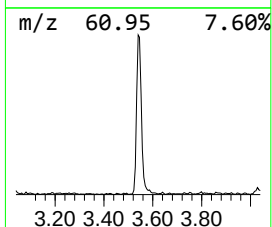
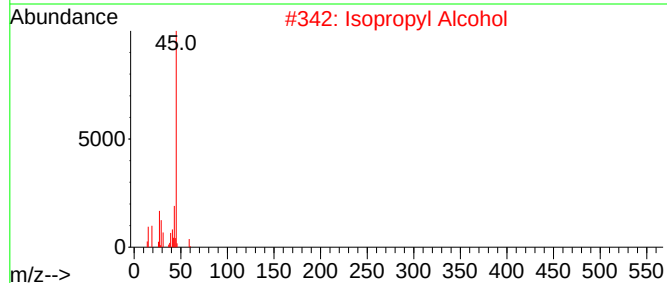
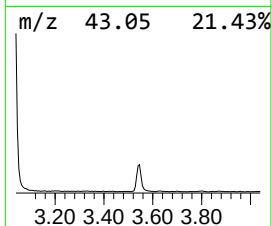
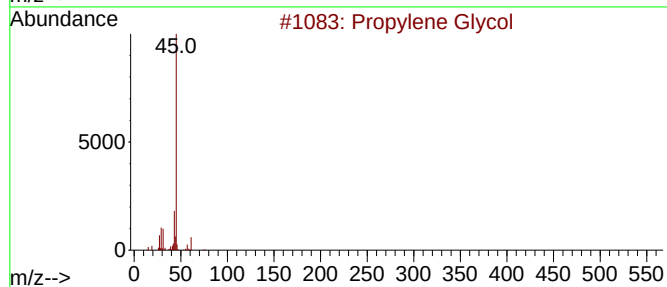
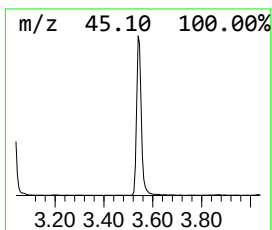
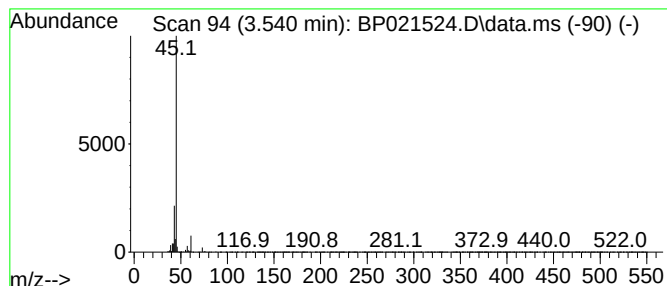
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Propylene Glycol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.540	3.60 ng	402775	1,4-Dichlorobenzene-d4	7.804

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propylene Glycol	76	C3H8O2	000057-55-6	90
2			Isopropyl Alcohol	60	C3H8O	000067-63-0	56
3			2-Pentanol, 4-methyl-	102	C6H14O	000108-11-2	17
4			2-Butanol, 3-methyl-	88	C5H12O	000598-75-4	9
5			R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	9



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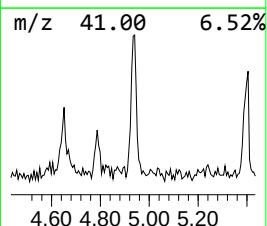
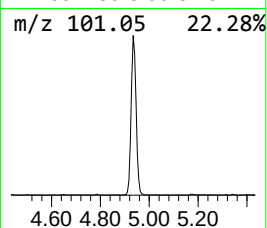
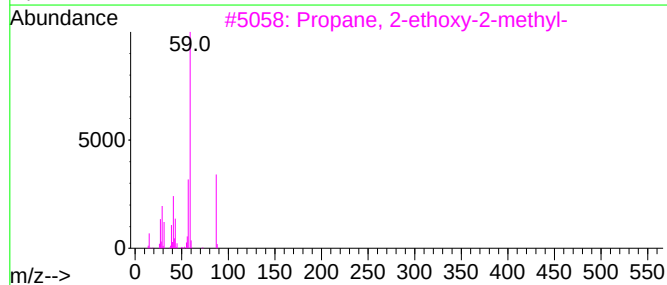
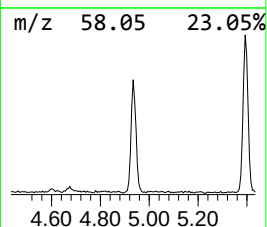
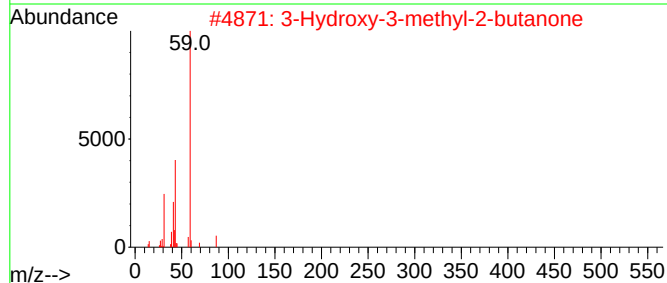
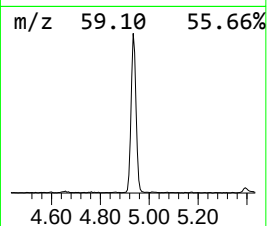
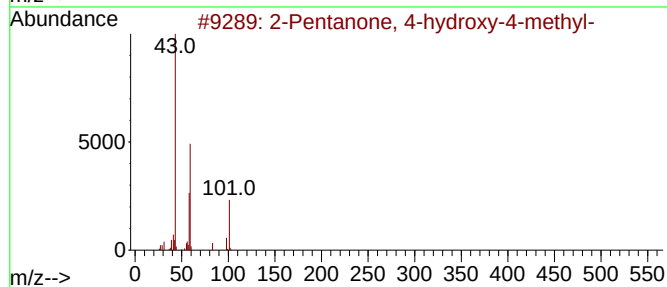
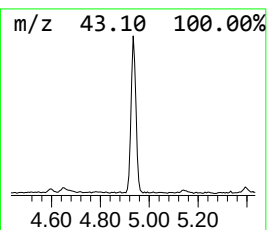
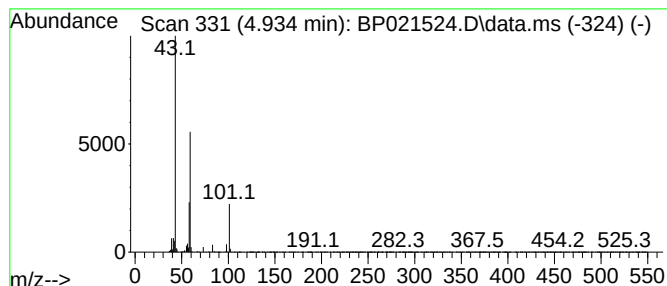
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.934	2.97 ng	332208	1,4-Dichlorobenzene-d4	7.804

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	47
2			3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	12
3			Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	12
4			Acetone	58	C3H6O	000067-64-1	12
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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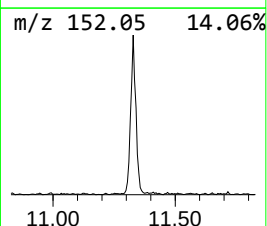
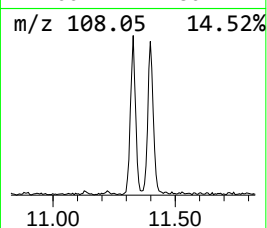
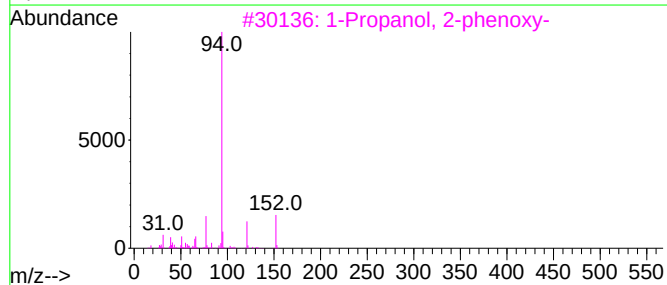
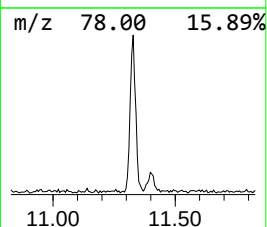
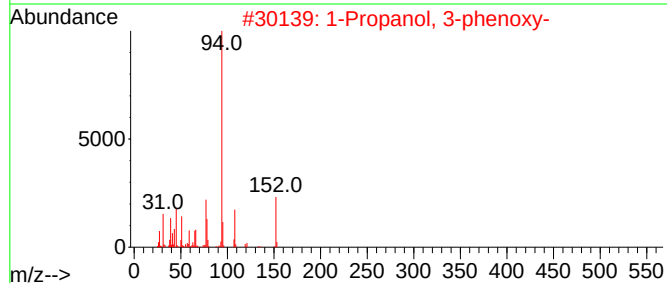
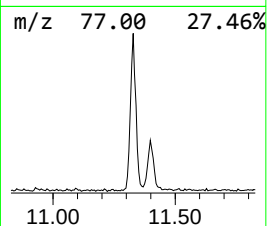
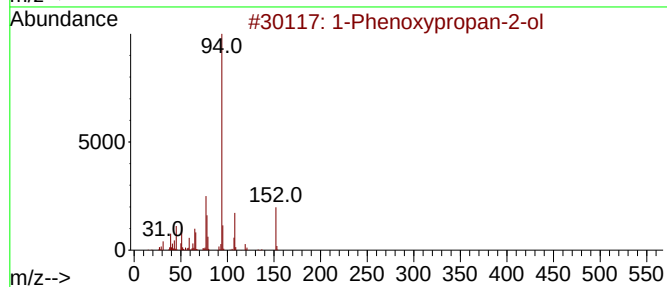
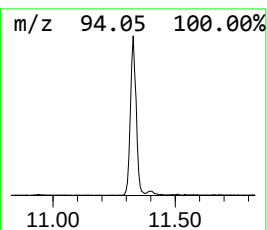
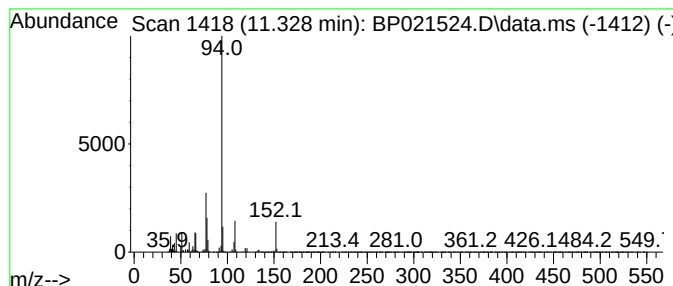
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Peak Number 4 1-Phenoxypropan-2-ol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.328	3.43 ng	505574	Naphthalene-d8	10.586

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	94
2			1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	83
3			1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	64
4			Carbonic acid, neopentyl phenyl ...	208	C12H16O3	013183-19-2	64
5			Benzene, (1-methylpropoxy)-	150	C10H14O	010574-17-1	53



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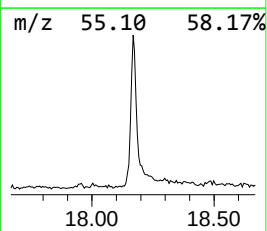
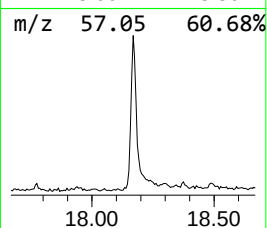
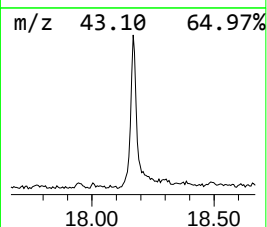
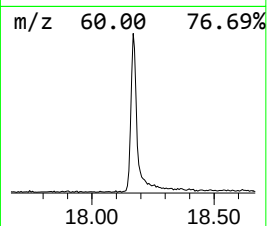
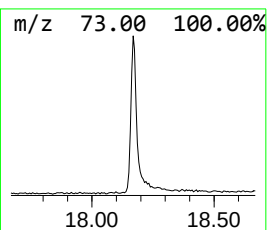
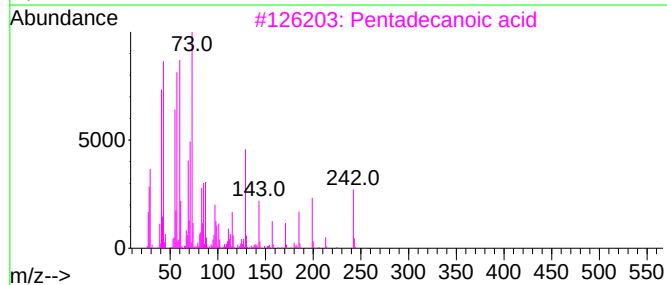
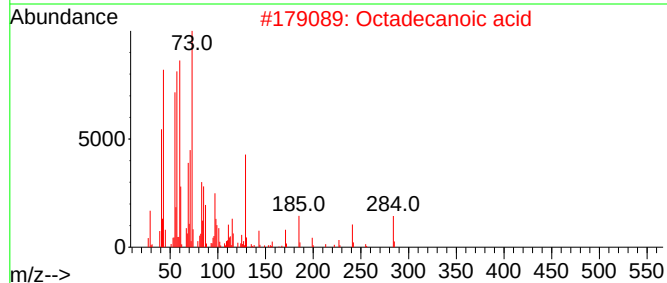
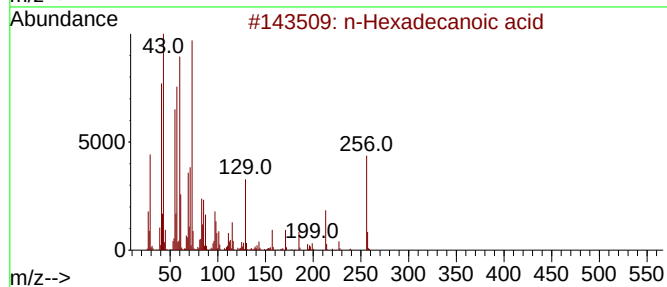
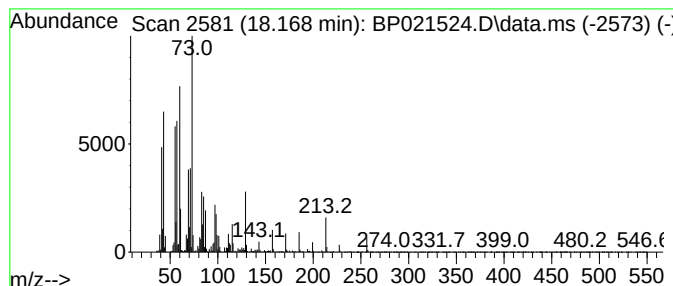
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.169	4.78 ng	1034210	Phenanthrene-d10	17.227

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2			Octadecanoic acid	284	C18H36O2	000057-11-4	91
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	80
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5			Isopropyl palmitate	298	C19H38O2	000142-91-6	58



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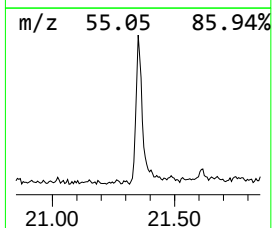
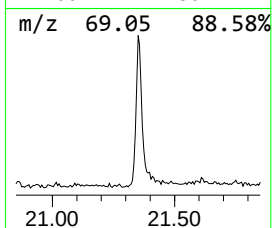
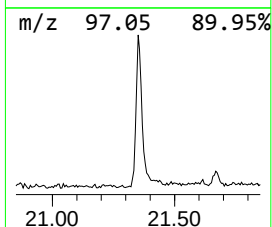
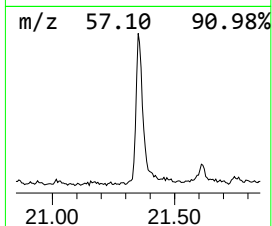
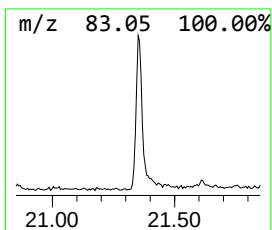
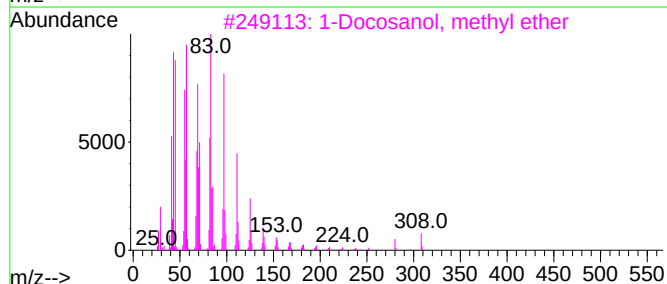
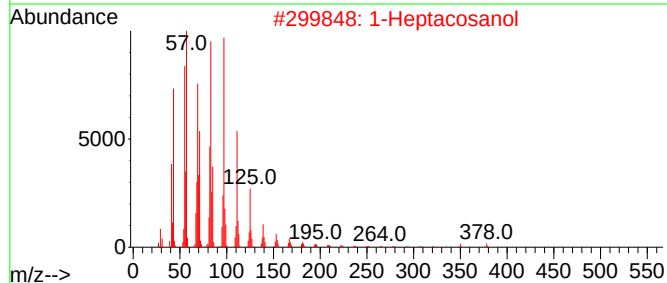
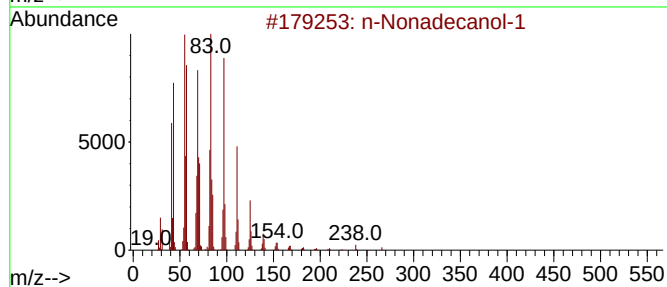
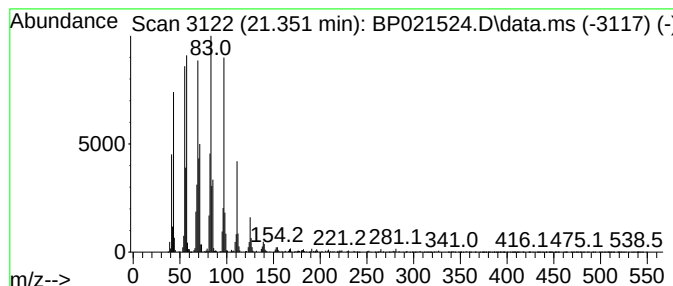
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 n-Nonadecanol-1 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.351	3.37 ng	850155	Chrysene-d12	21.668

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Nonadecanol-1	284	C19H40O	001454-84-8	91
2		1-Heptacosanol	396	C27H56O	002004-39-9	91
3		1-Docosanol, methyl ether	340	C23H48O	1000333-91-9	91
4		1-Heneicosanol	312	C21H44O	015594-90-8	91
5		Isoheptadecanol	256	C17H36O	057289-07-3	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP081524\
Data File : BP021524.D
Acq On : 15 Aug 2024 22:14
Operator : RC/JU
Sample : P3573-10
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
S-856-J-S0-4-4.5-080924

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP081324.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
Butane, 2-metho...	3.028	44.9	ng	5024740	1	7.804	2238670	20.0
Propylene Glycol	3.540	3.6	ng	402775	1	7.804	2238670	20.0
2-Pentanone, 4-...	4.934	3.0	ng	332208	1	7.804	2238670	20.0
1-Phenoxypropan...	11.328	3.4	ng	505574	2	10.586	2946290	20.0
n-Hexadecanoic ...	18.169	4.8	ng	1034210	4	17.227	4327100	20.0
n-Nonadecanol-1	21.351	3.4	ng	850155	5	21.668	5051160	20.0