

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP082224\
 Data File : BP021615.D
 Acq On : 22 Aug 2024 15:48
 Operator : RC/JU
 Sample : P3689-02
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 WC-1

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: BP021615.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	20	rVB	4358333	5450848	36.07%	6.196%
2	3.546	90	95	106	rBV	289881	391221	2.59%	0.445%
3	4.934	325	331	343	rBV	256555	384587	2.54%	0.437%
4	5.393	402	409	422	rBV	4749254	7227424	47.83%	8.215%
5	6.964	668	676	691	rBV	4832923	7752269	51.30%	8.812%
6	7.399	745	750	759	rBV	101977	169923	1.12%	0.193%
7	7.799	811	818	824	rBV	1027021	1682263	11.13%	1.912%
8	8.946	1005	1013	1026	rBV	2617034	4695625	31.07%	5.337%
9	9.505	1102	1108	1117	rBV	142844	212210	1.40%	0.241%
10	10.587	1284	1292	1306	rBV	1247131	2403594	15.91%	2.732%
11	11.328	1411	1418	1429	rBV	295579	591765	3.92%	0.673%
12	13.057	1703	1712	1723	rBV	5407038	9039819	59.82%	10.275%
13	14.451	1940	1949	1958	rBV	1954824	3440318	22.77%	3.910%
14	14.675	1985	1987	1994	rVB	152636	190972	1.26%	0.217%
15	15.969	2195	2207	2216	rBV	5694371	9487953	62.78%	10.785%
16	17.263	2420	2427	2432	rBV	3315392	4601110	30.45%	5.230%
17	17.392	2444	2449	2453	rVB	117782	164308	1.09%	0.187%
18	18.198	2577	2586	2598	rBV2	578994	1190676	7.88%	1.353%
19	19.086	2732	2737	2742	rBV2	96765	188230	1.25%	0.214%
20	19.386	2783	2788	2794	rBV	215266	384151	2.54%	0.437%
21	19.533	2809	2813	2821	rVV	293005	436181	2.89%	0.496%
22	19.769	2848	2853	2859	rBV2	254675	554461	3.67%	0.630%
23	19.980	2883	2889	2900	rVB	10042665	15111926	100.00%	17.177%
24	21.398	3125	3130	3140	rBV	865914	1362189	9.01%	1.548%
25	21.722	3179	3185	3191	rBV2	3383880	5452310	36.08%	6.197%
26	25.157	3761	3769	3782	rVB	1989526	5411249	35.81%	6.151%

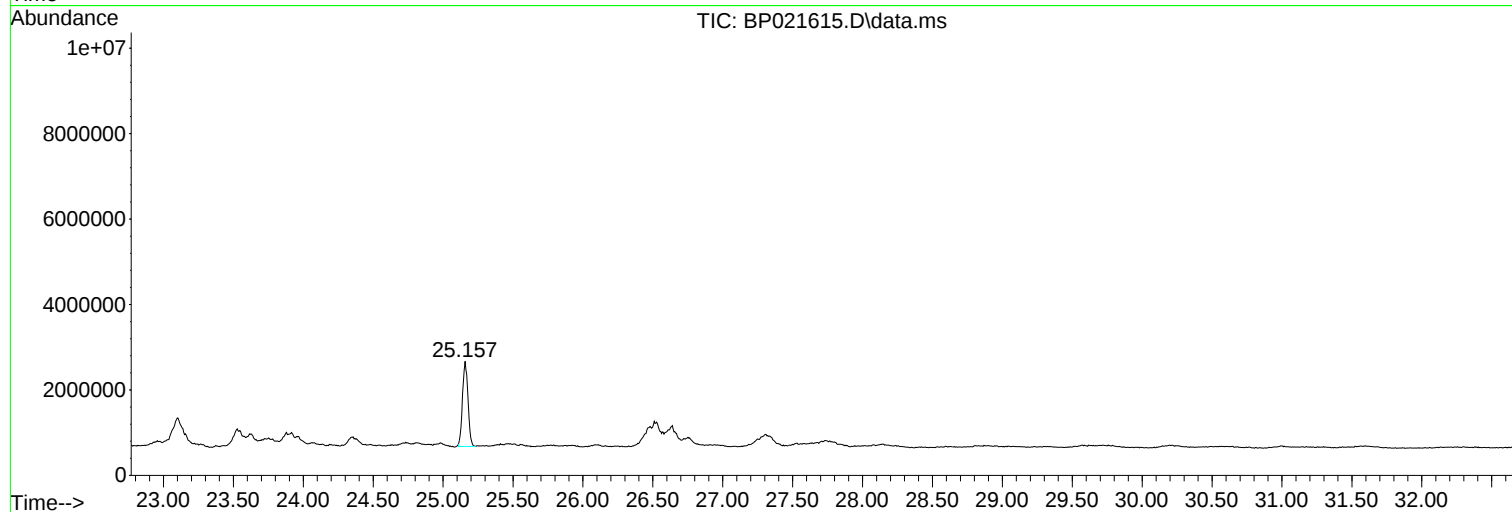
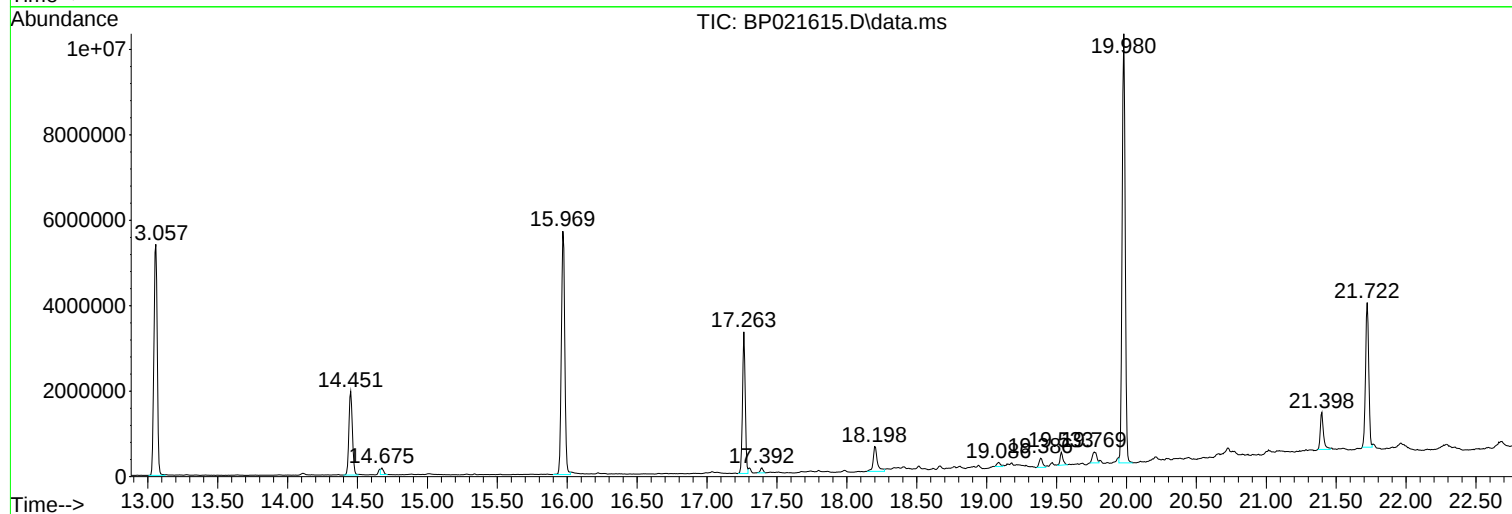
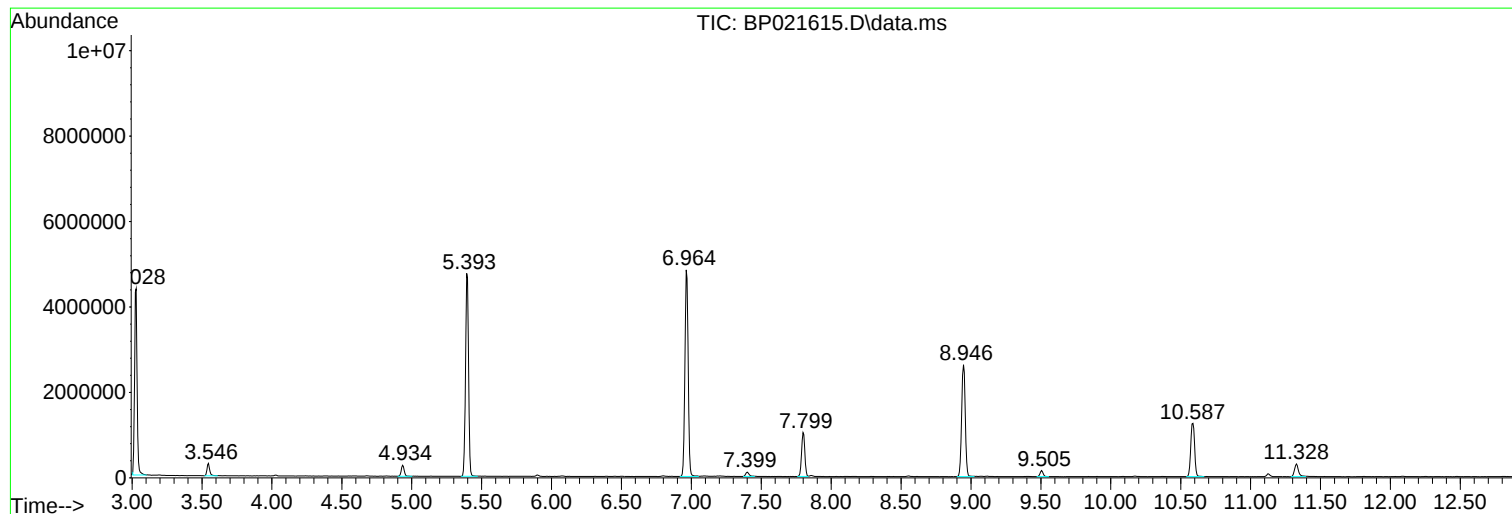
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP081324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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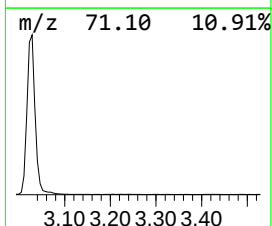
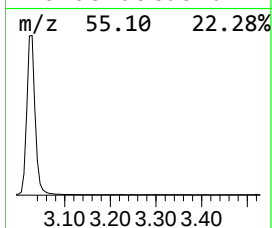
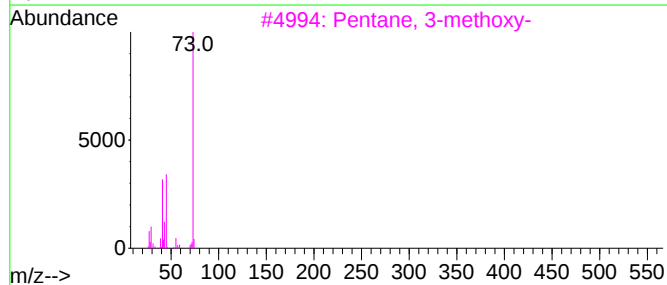
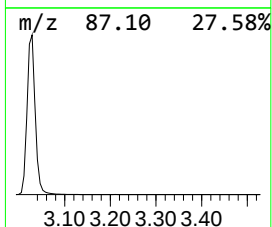
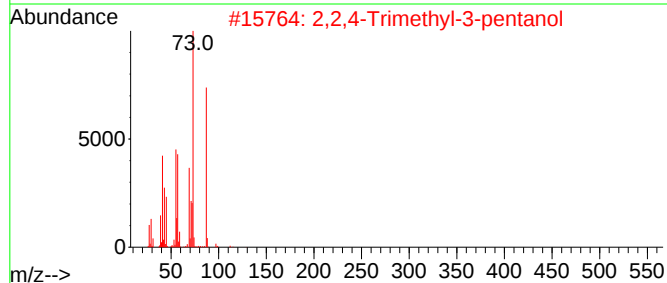
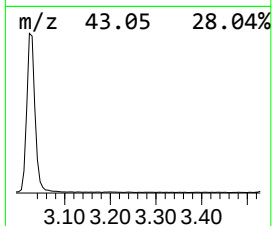
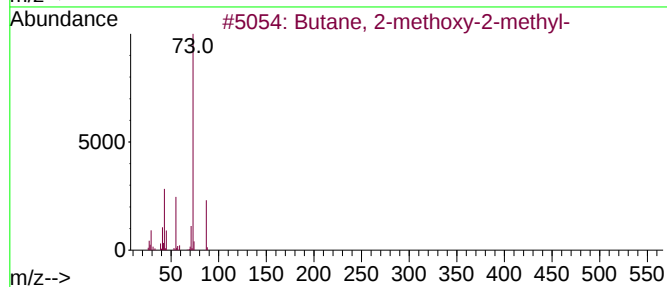
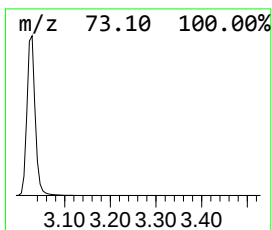
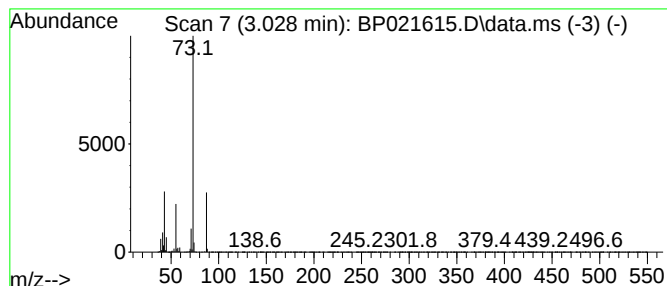
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	64.80 ng	5450850	1,4-Dichlorobenzene-d4	7.799

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	86
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4			Borane, dimethoxy-	74	C2H7B02	004542-61-4	9
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9



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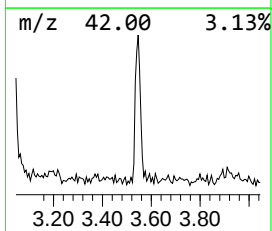
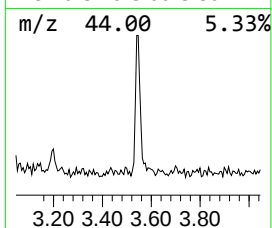
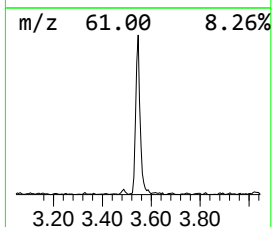
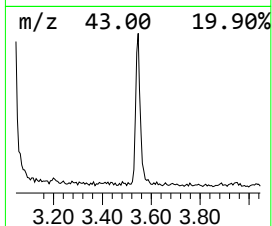
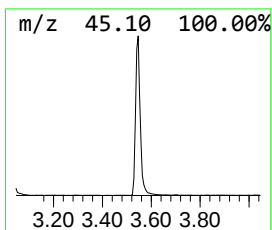
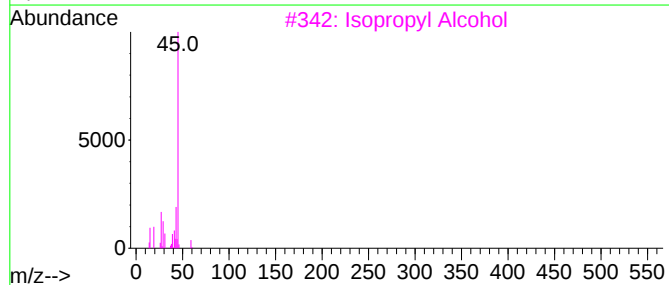
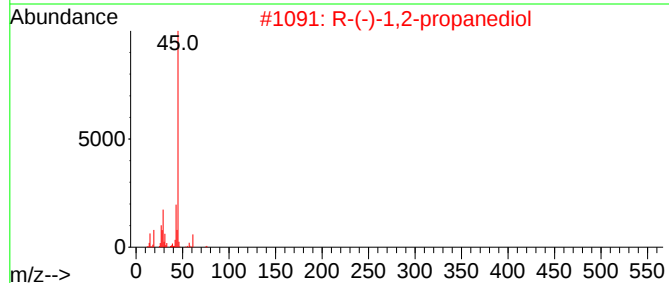
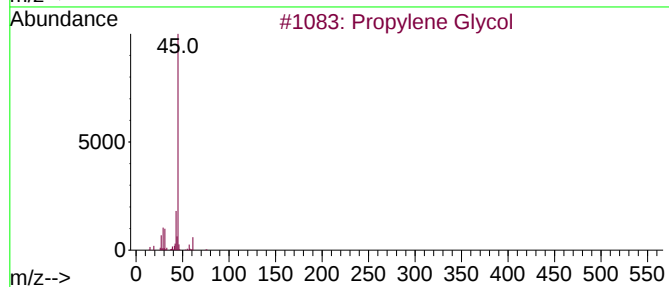
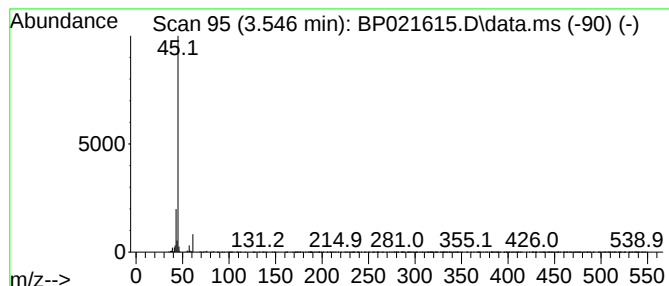
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Propylene Glycol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.546	4.65 ng	391221	1,4-Dichlorobenzene-d4	7.799

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propylene Glycol	76	C3H8O2	000057-55-6	86
2			R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	64
3			Isopropyl Alcohol	60	C3H8O	000067-63-0	50
4			Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	40
5			2-Butanol, 3-methyl-	88	C5H12O	000598-75-4	9



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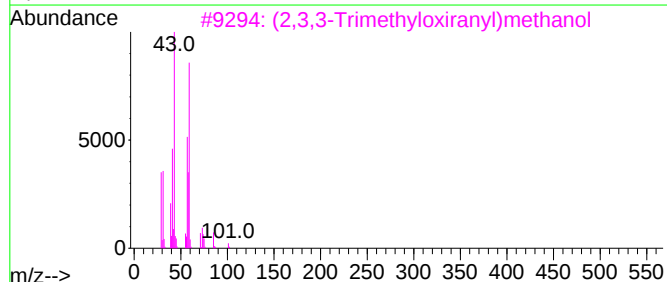
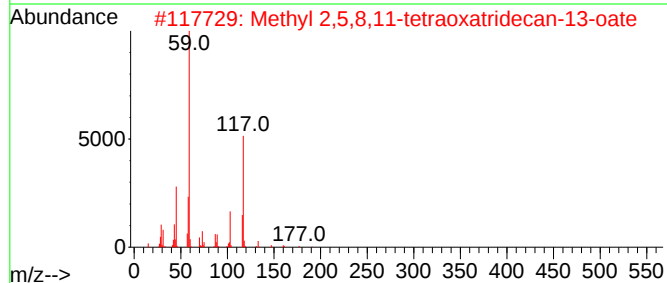
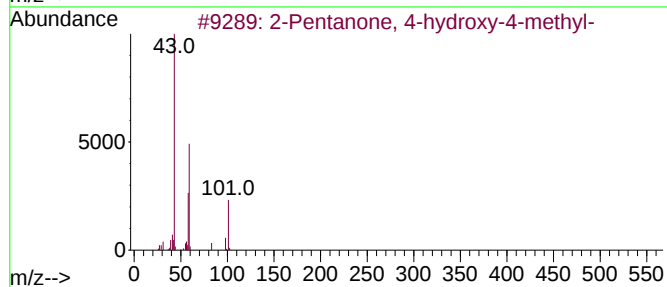
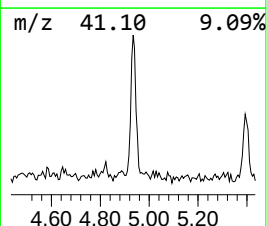
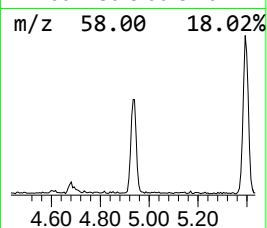
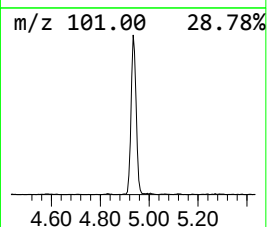
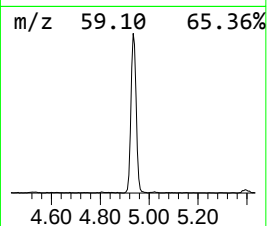
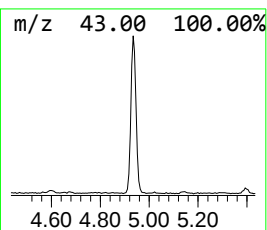
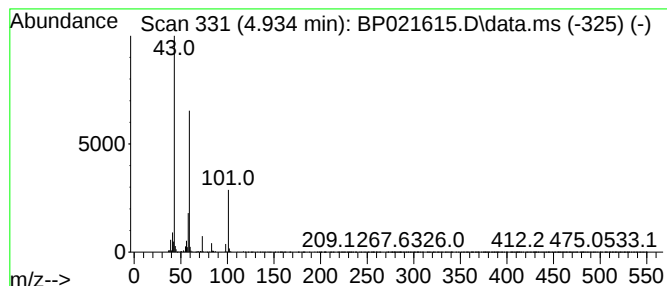
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.934	4.57 ng	384587	1,4-Dichlorobenzene-d4	7.799

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Methyl 2,5,8,11-tetraoxatridecan...	236	C10H20O6	1000366-78-2	37
3			(2,3,3-Trimethyloxiranyl)methanol	116	C6H12O2	1000306-64-7	33
4			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	25
5			2-Butanol, 1-methoxy-	104	C5H12O2	053778-73-7	23



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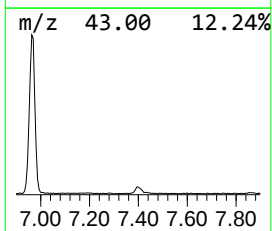
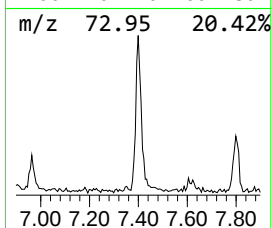
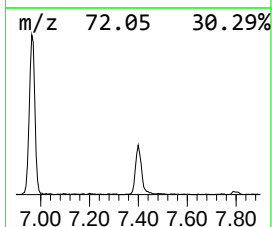
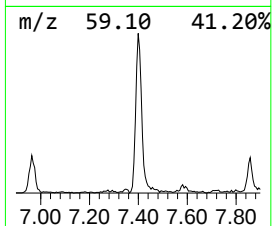
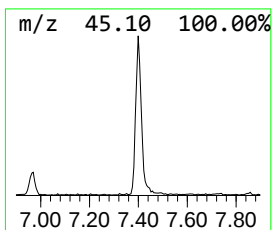
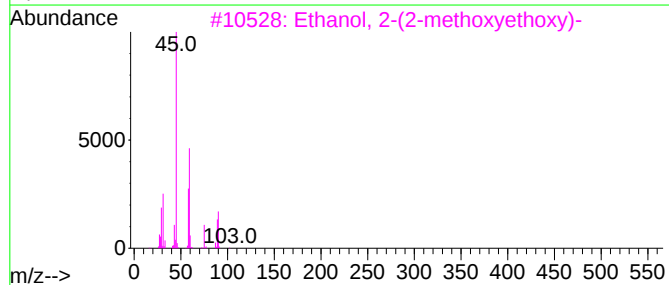
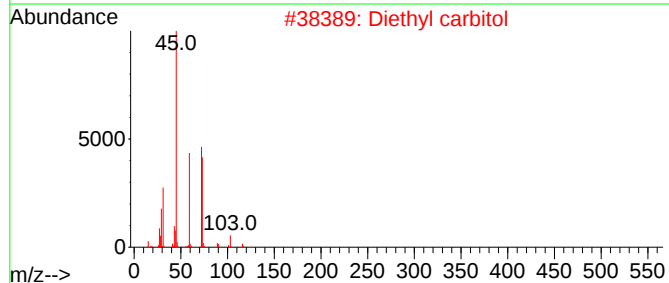
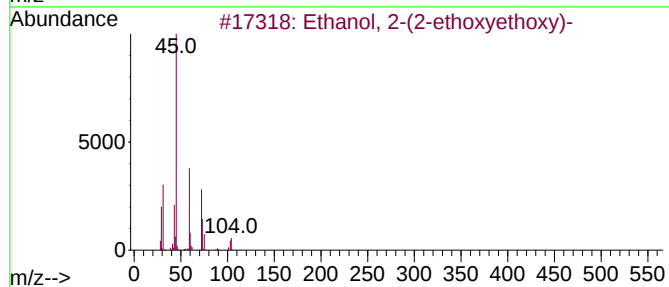
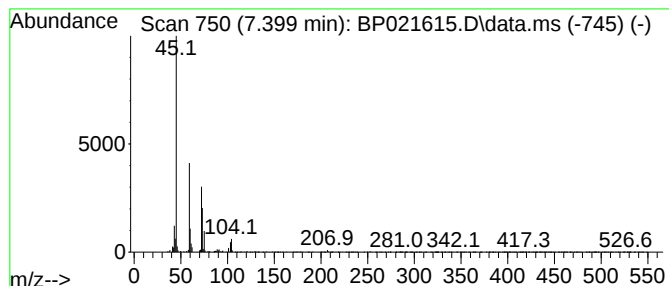
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Peak Number 4 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.399	2.02 ng	169923	1,4-Dichlorobenzene-d4	7.799

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	90
2			Diethyl carbitol	162	C8H18O3	000112-36-7	64
3			Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	53
4			2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	50
5			Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	45



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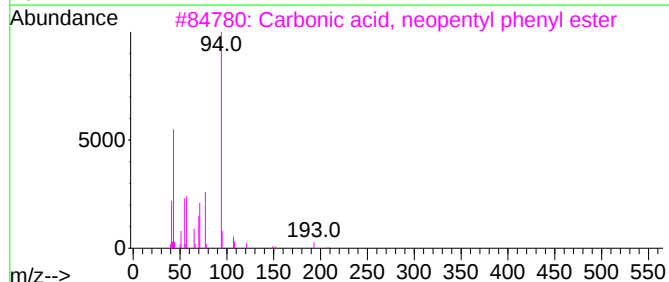
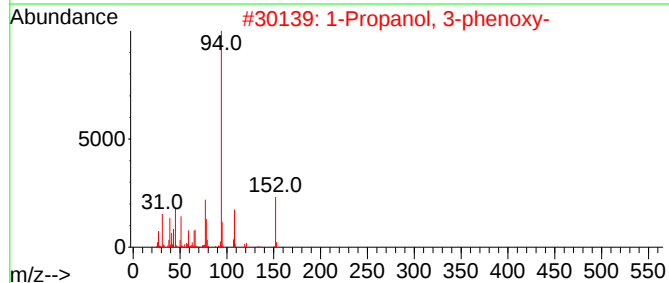
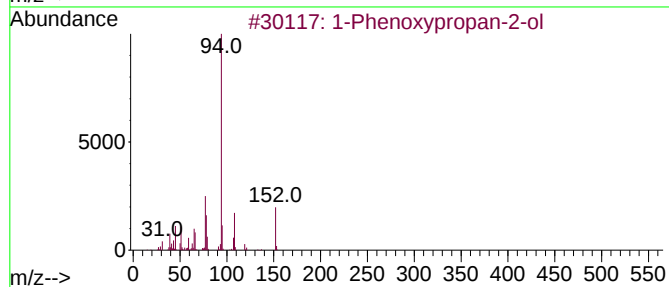
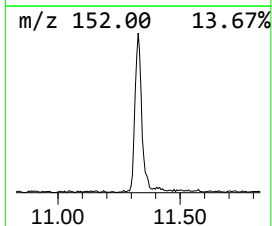
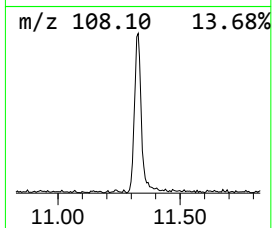
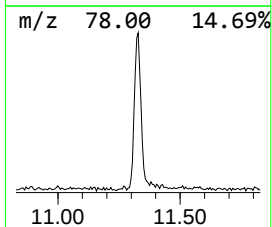
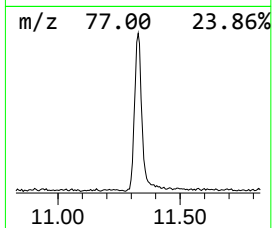
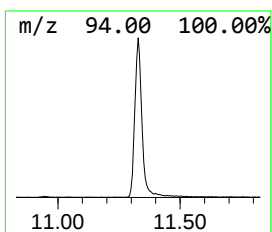
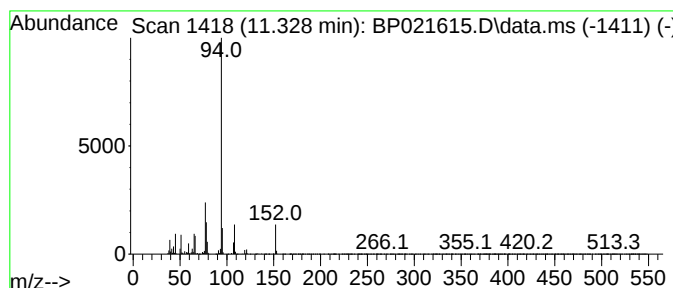
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 1-Phenoxypropan-2-ol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.328	4.92 ng	591765	Naphthalene-d8	10.587

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	96
2			1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	83
3			Carbonic acid, neopentyl phenyl ...	208	C12H16O3	013183-19-2	64
4			1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	64
5			Ethanethiol, 2-phenoxy-	154	C8H10OS	006338-63-2	53



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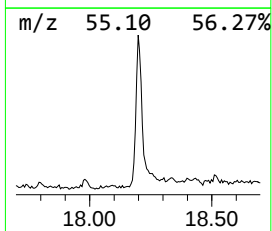
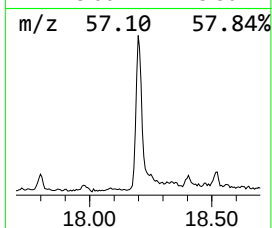
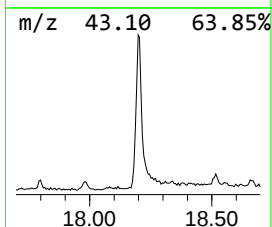
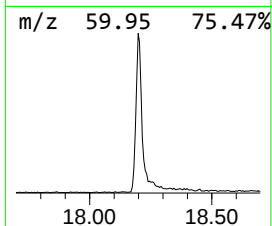
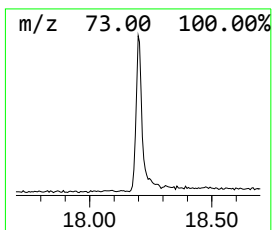
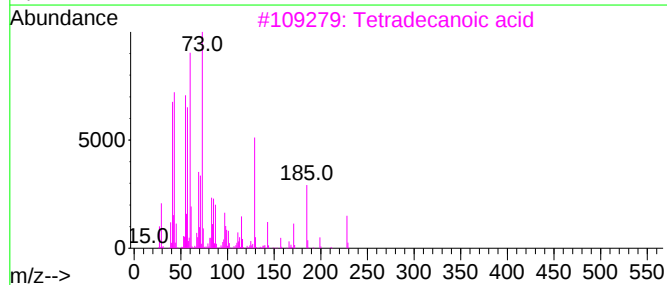
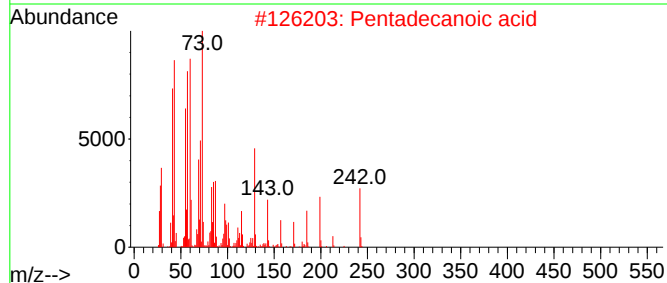
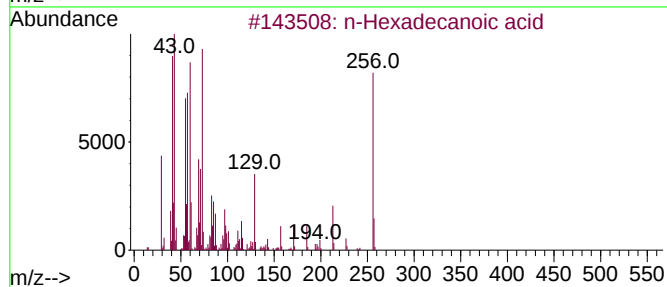
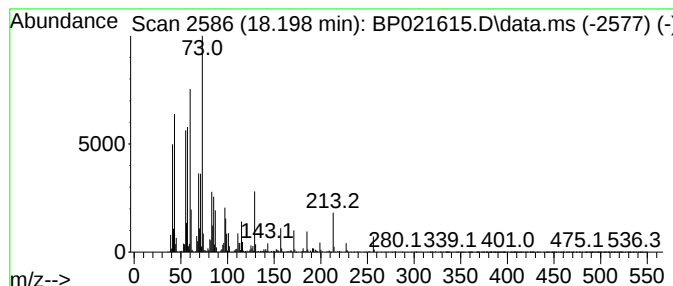
Instrument :
BNA_P
ClientSampleId :
WC-1

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

Peak Number 6 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.198	5.18 ng	1190680	Phenanthrene-d10	17.263	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4	Tridecanoic acid	214	C13H26O2	000638-53-9	59
5	Dodecanoic acid	200	C12H24O2	000143-07-7	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP082224\
Data File : BP021615.D
Acq On : 22 Aug 2024 15:48
Operator : RC/JU
Sample : P3689-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
WC-1

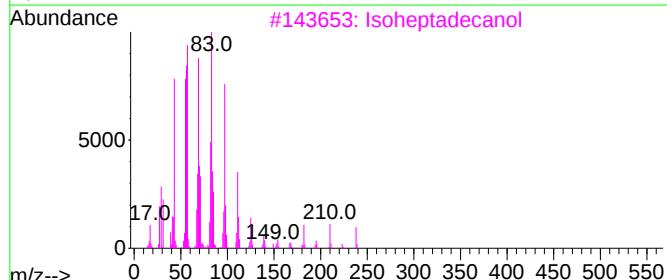
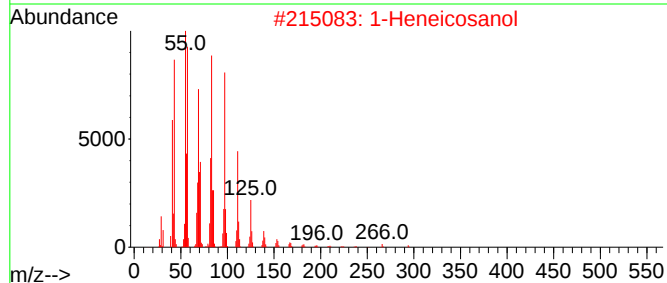
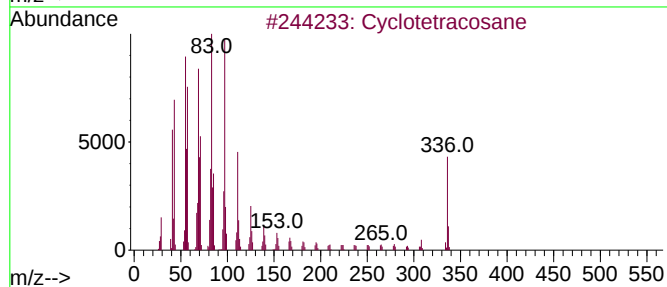
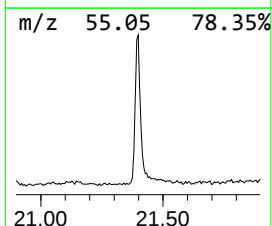
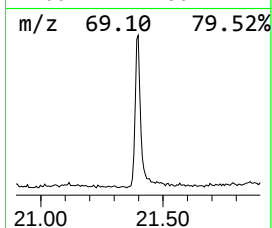
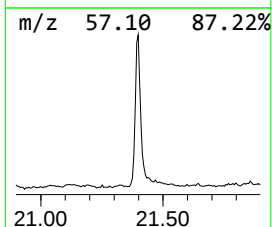
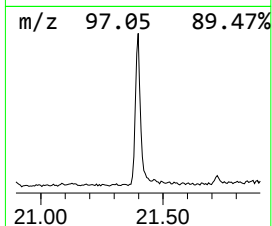
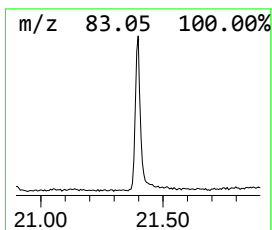
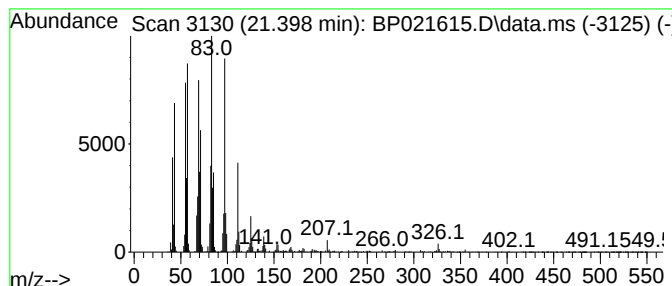
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Cyclotetracosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.398	5.00 ng	1362190	Chrysene-d12	21.722

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclotetracosane	336	C24H48	000297-03-0	97
2			1-Heneicosanol	312	C21H44O	015594-90-8	90
3			Isoheptadecanol	256	C17H36O	057289-07-3	87
4			Behenic alcohol	326	C22H46O	000661-19-8	87
5			1-Hexacosanol	382	C26H54O	000506-52-5	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP082224\
Data File : BP021615.D
Acq On : 22 Aug 2024 15:48
Operator : RC/JU
Sample : P3689-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
WC-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP081324.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
Butane, 2-metho...	3.028	64.8	ng	5450850	1	7.799	1682260	20.0
Propylene Glycol	3.546	4.7	ng	391221	1	7.799	1682260	20.0
2-Pentanone, 4-...	4.934	4.6	ng	384587	1	7.799	1682260	20.0
Ethanol, 2-(2-e...	7.399	2.0	ng	169923	1	7.799	1682260	20.0
1-Phenoxypropan...	11.328	4.9	ng	591765	2	10.587	2403590	20.0
n-Hexadecanoic ...	18.198	5.2	ng	1190680	4	17.263	4601110	20.0
Cyclotetracosane	21.398	5.0	ng	1362190	5	21.722	5452310	20.0