

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP082024\
 Data File : BP021578.D
 Acq On : 20 Aug 2024 18:51
 Operator : RC/JU
 Sample : P3643-12
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 921-J-SD-0.5-1.0-081524

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: BP021578.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	22	rVB	3962535	4881297	33.72%	5.703%
2	3.546	90	95	105	rBV	172257	241113	1.67%	0.282%
3	4.934	326	331	337	rBV	247996	360292	2.49%	0.421%
4	5.399	403	410	423	rBV	4443793	6648377	45.93%	7.768%
5	6.969	669	677	690	rBV	4226110	6999463	48.36%	8.178%
6	7.804	812	819	825	rBV	1283381	1980445	13.68%	2.314%
7	8.951	1004	1014	1027	rBV	2577684	4283415	29.59%	5.004%
8	9.510	1104	1109	1116	rBV	122748	192283	1.33%	0.225%
9	10.593	1284	1293	1307	rBV	1503631	2776896	19.18%	3.244%
10	11.334	1412	1419	1426	rBV	243972	473152	3.27%	0.553%
11	13.063	1705	1713	1727	rBV	5952641	8454127	58.40%	9.877%
12	14.457	1940	1950	1957	rBV	2741472	3929065	27.14%	4.590%
13	14.681	1979	1988	2002	rBV3	803548	2136928	14.76%	2.497%
14	15.969	2201	2207	2217	rBV	5507376	8143631	56.26%	9.515%
15	17.269	2421	2428	2434	rBV	3353228	5130030	35.44%	5.994%
16	18.216	2583	2589	2598	rBV	490027	752908	5.20%	0.880%
17	19.204	2753	2757	2764	rVB4	128198	177889	1.23%	0.208%
18	19.398	2786	2790	2798	rBV	96485	167257	1.16%	0.195%
19	19.545	2812	2815	2820	rBV3	141387	204546	1.41%	0.239%
20	19.998	2886	2892	2899	rVB	9813002	14475026	100.00%	16.912%
21	21.404	3127	3131	3140	rBV	993708	1424693	9.84%	1.665%
22	21.733	3180	3187	3193	rBV	3708402	5881371	40.63%	6.871%
23	25.168	3763	3771	3784	rVB	2117615	5877505	40.60%	6.867%

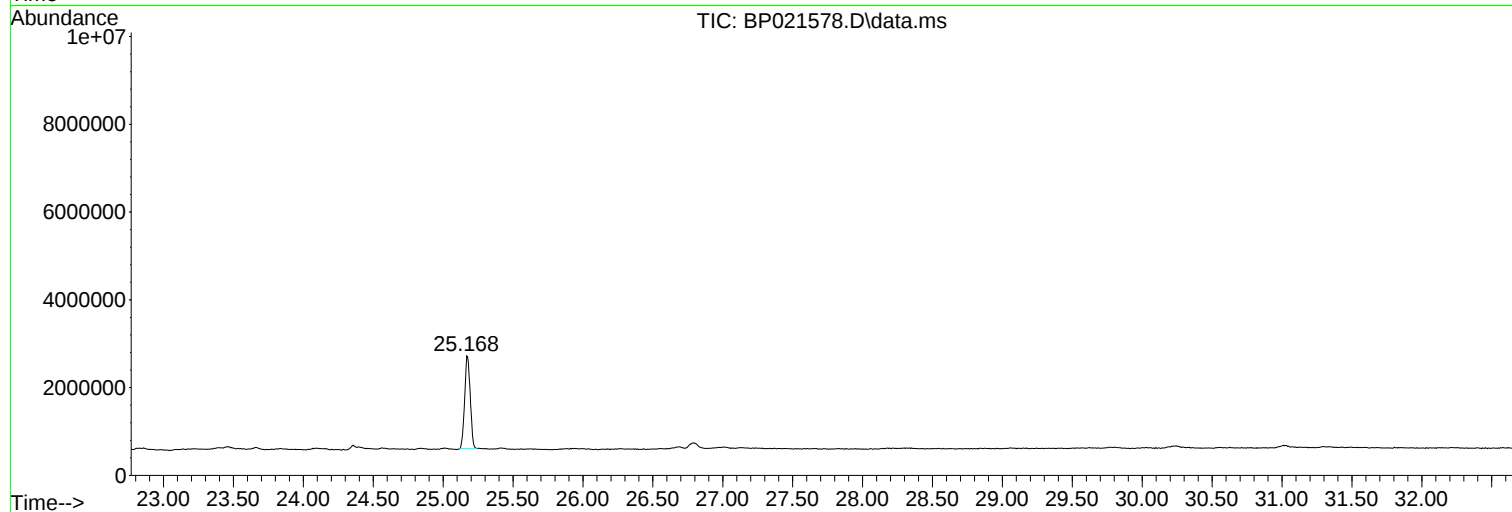
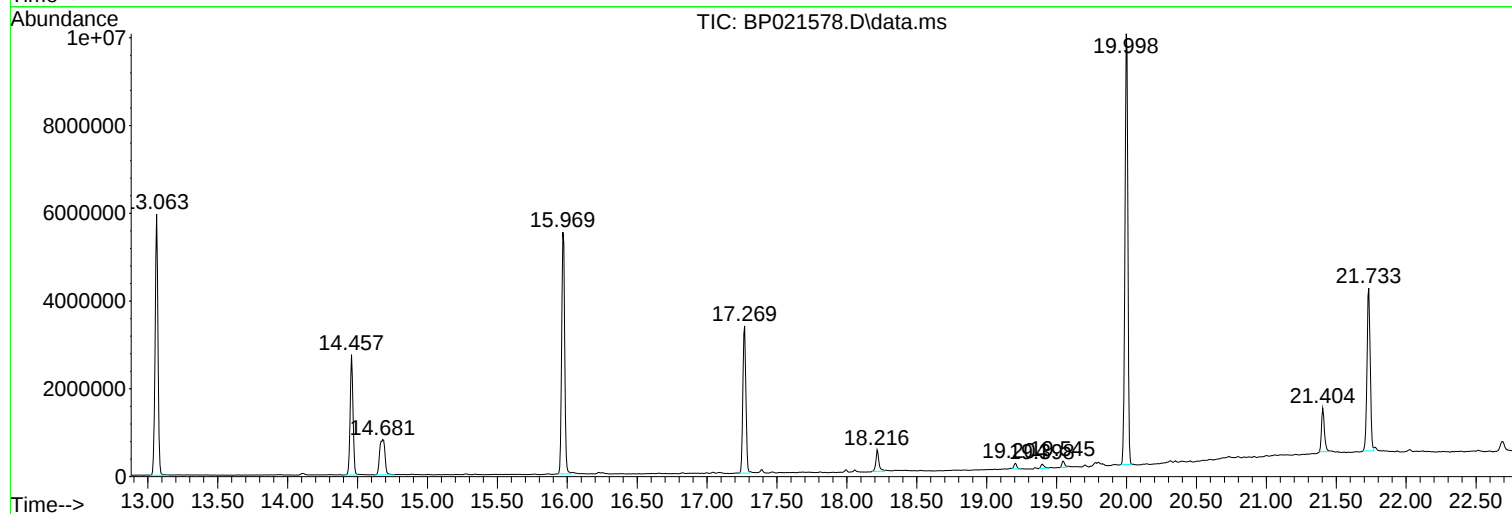
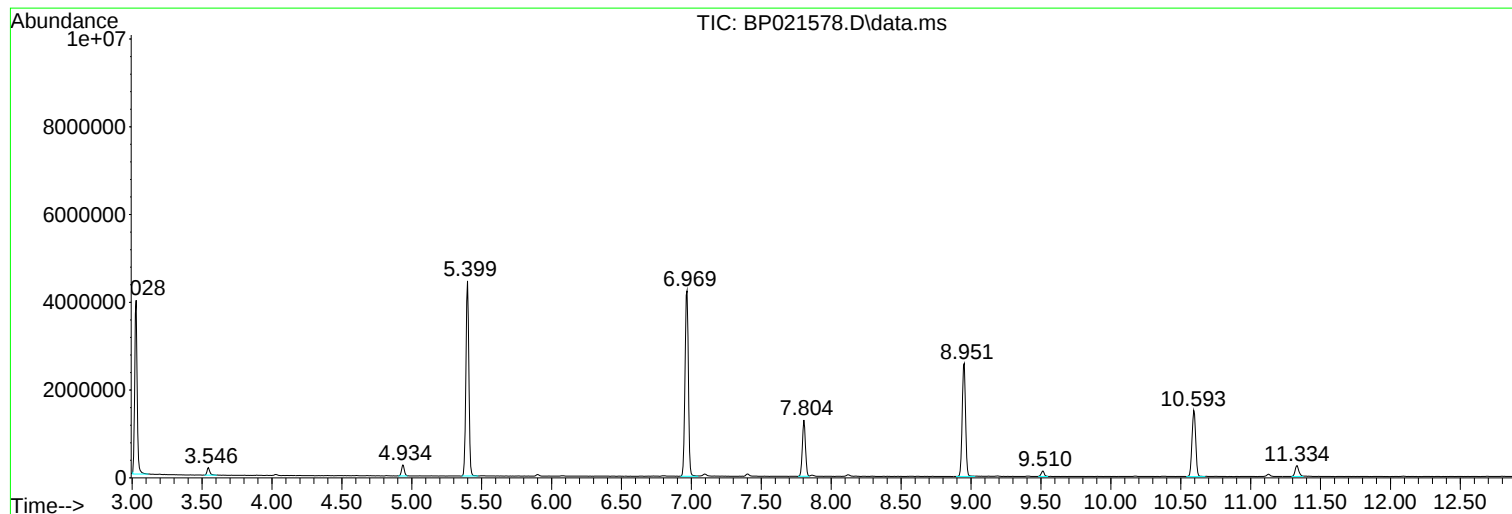
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP081324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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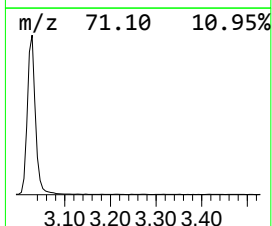
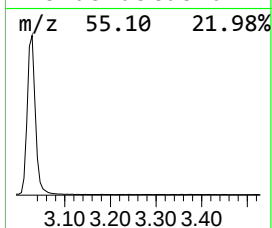
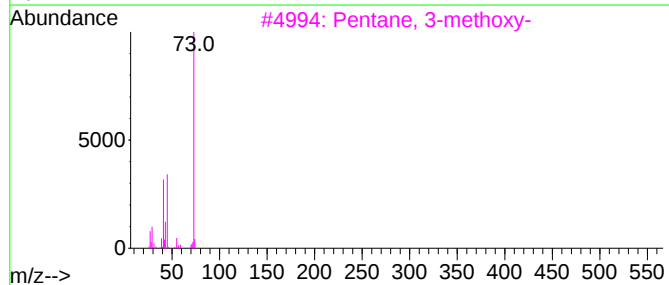
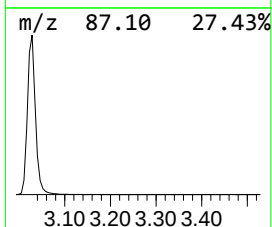
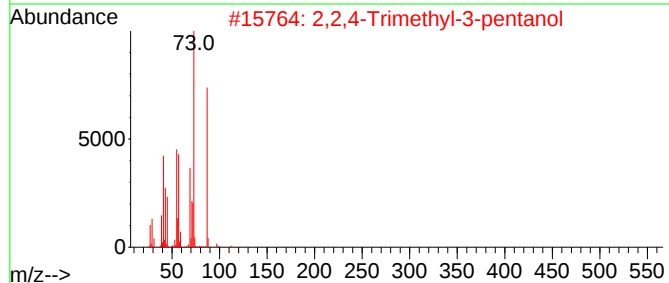
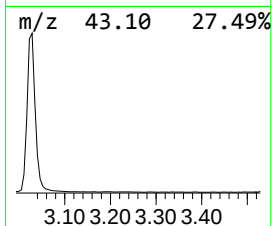
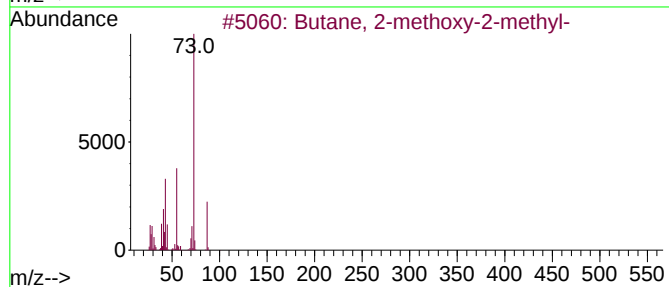
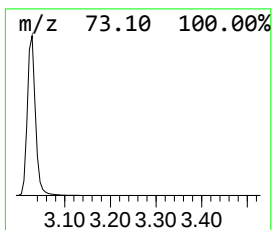
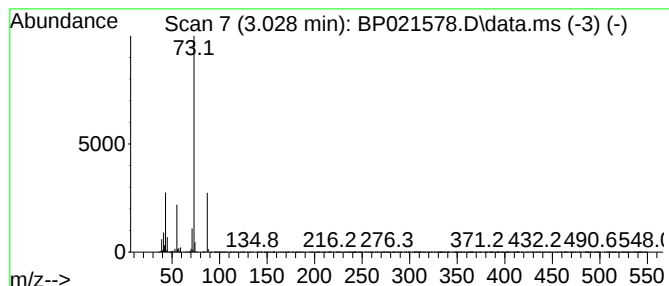
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	49.30 ng	4881300	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			Silane, tetramethyl-	88	C4H12Si	000075-76-3	9



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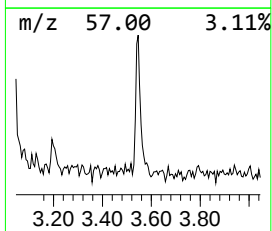
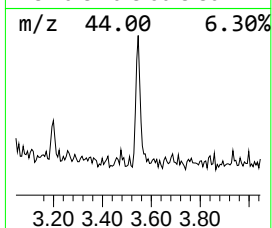
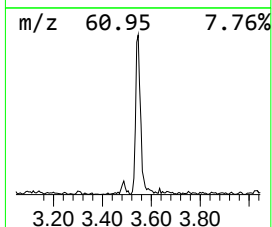
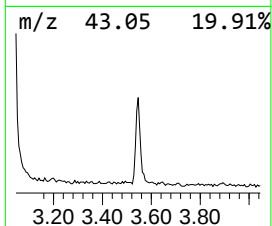
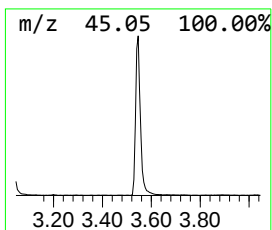
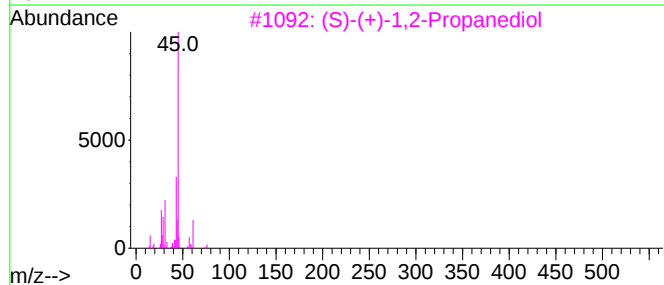
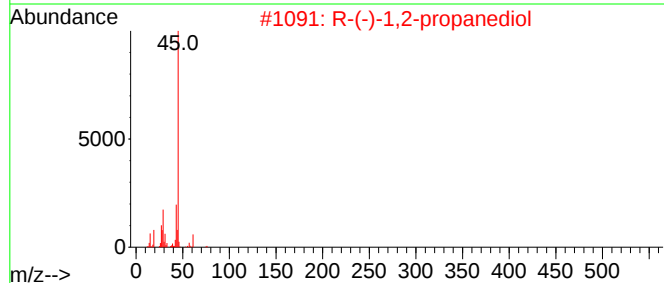
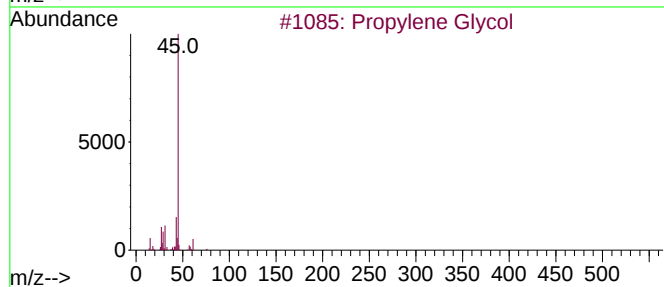
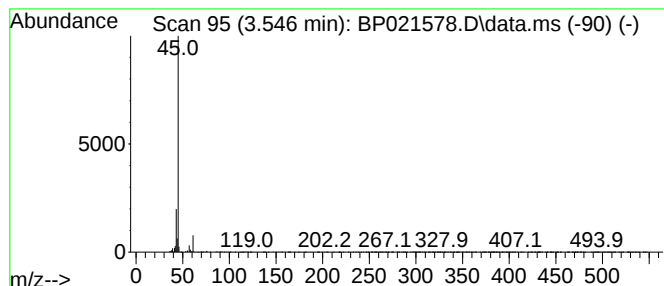
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Propylene Glycol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.546	2.43 ng	241113	1,4-Dichlorobenzene-d4	7.804

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propylene Glycol	76	C3H8O2	000057-55-6	78
2			R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	72
3			(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	12
4			Isopropyl Alcohol	60	C3H8O	000067-63-0	9
5			2-Pentanol	88	C5H12O	006032-29-7	9



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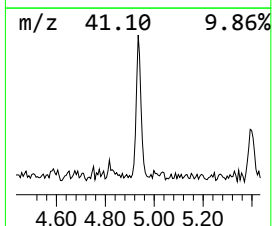
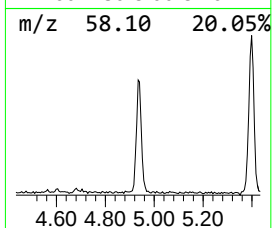
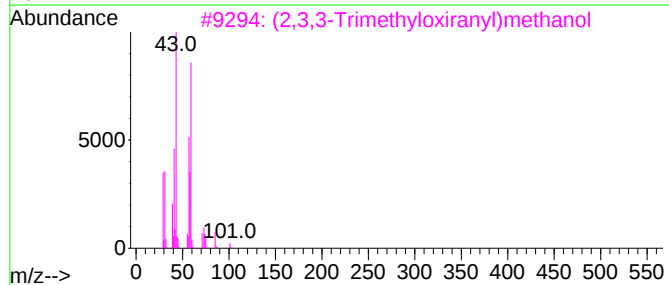
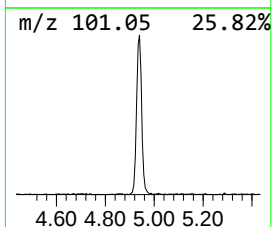
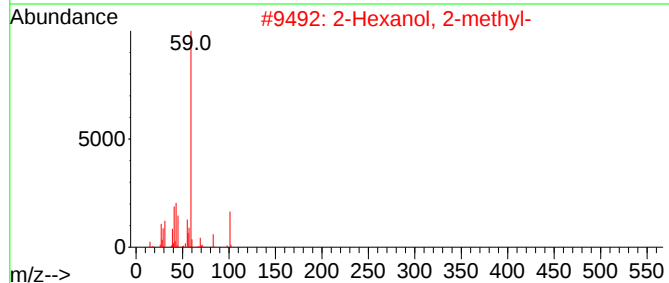
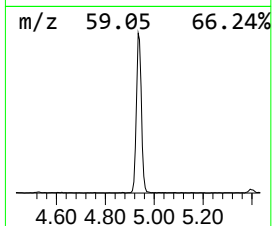
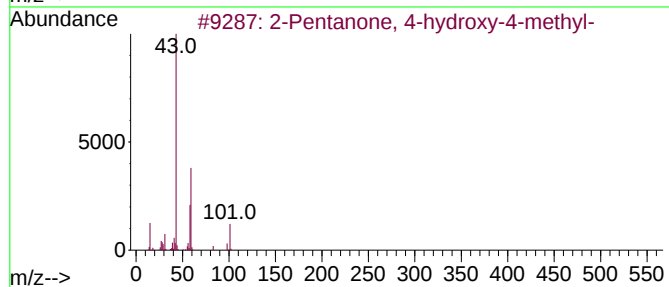
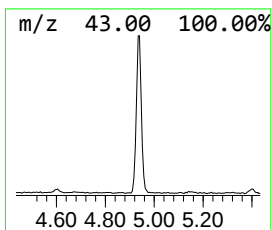
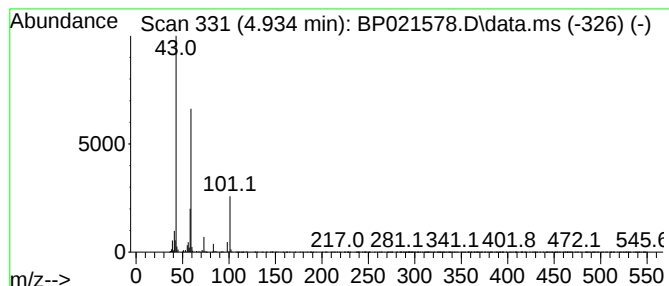
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.934	3.64 ng	360292	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	53
2			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	38
3			(2,3,3-Trimethyloxiranyl)methanol	116	C6H12O2	1000306-64-7	33
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	18
5			2-Propanol, 1-(2-methoxypropoxy)-	148	C7H16O3	013429-07-7	17



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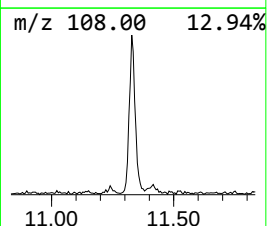
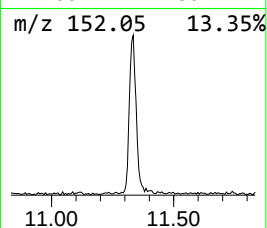
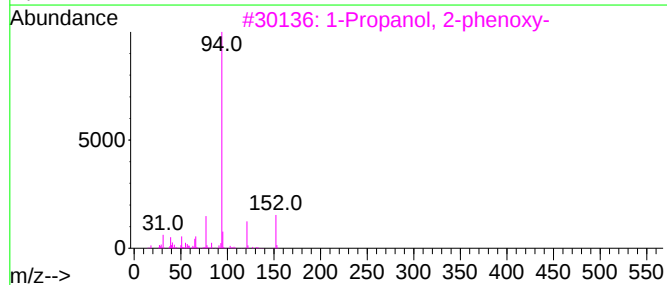
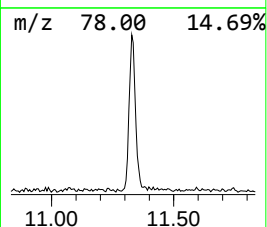
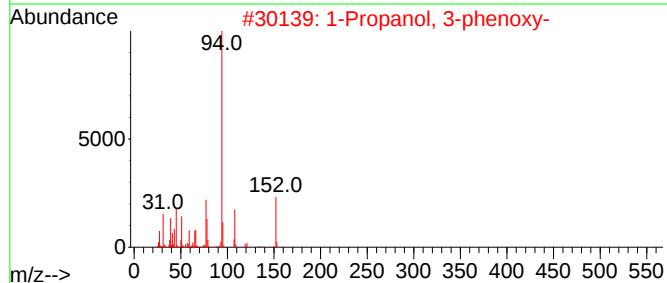
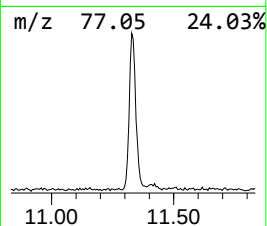
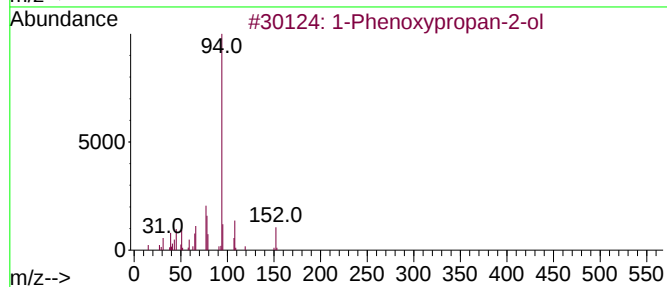
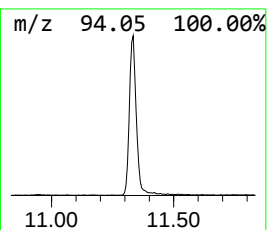
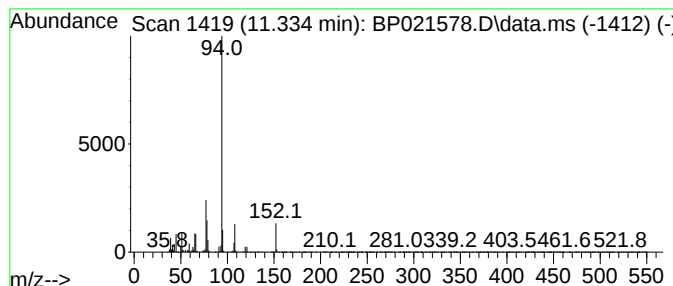
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Peak Number 4 1-Phenoxypropan-2-ol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.334	3.41 ng	473152	Naphthalene-d8	10.593

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	90
3			1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	64
4			Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	59
5			Benzene, (2-methylpropoxy)-	150	C10H14O	001126-75-6	58



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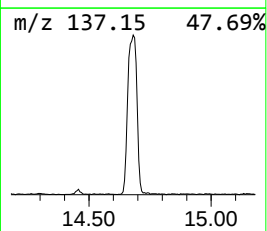
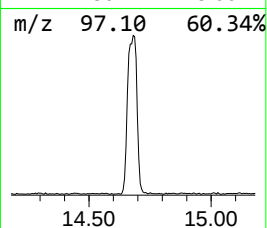
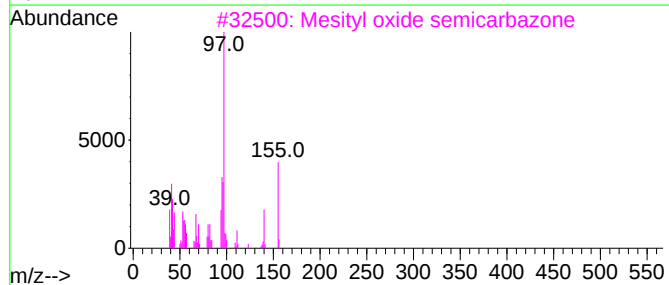
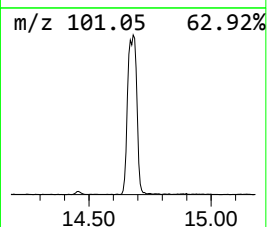
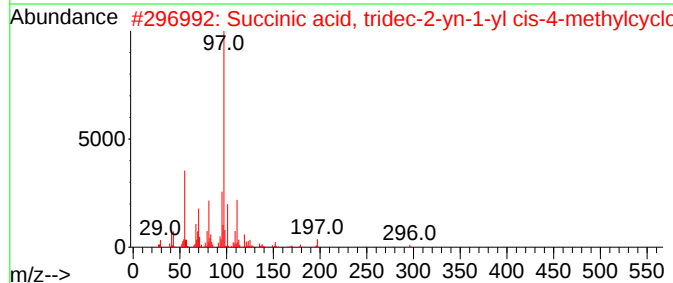
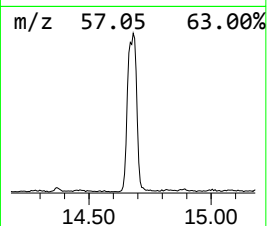
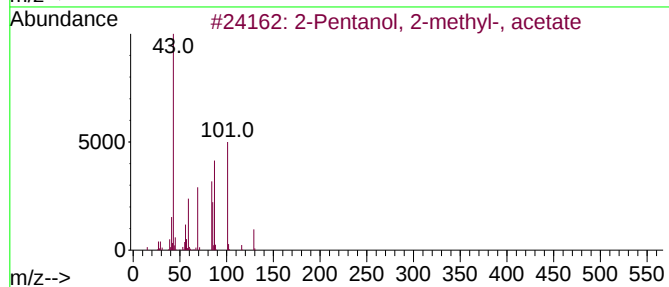
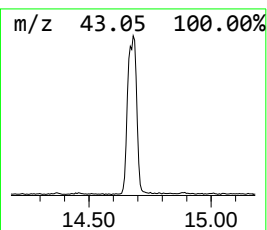
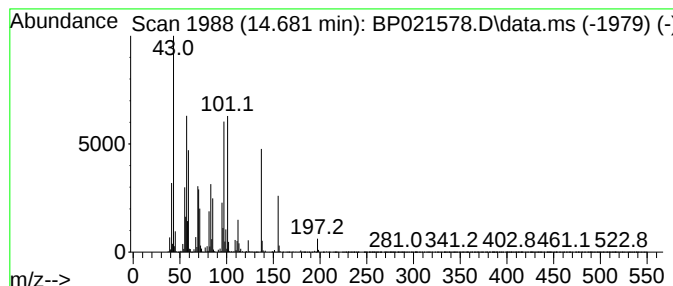
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 unknown14.681 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.681	10.88 ng	2136930	Acenaphthene-d10	14.457

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanol, 2-methyl-, acetate	144	C8H16O2	034859-98-8	14
2			Succinic acid, tridec-2-yn-1-yl ...	392	C24H40O4	1000390-06-3	14
3			Mesityl oxide semicarbazone	155	C7H13N3O	003780-62-9	14
4			1-(2-Furyl)-3-buten-1-ol	138	C8H10O2	1000311-94-9	11
5			Cyclohexane, 1,3-dimethyl-, cis-	112	C8H16	000638-04-0	11



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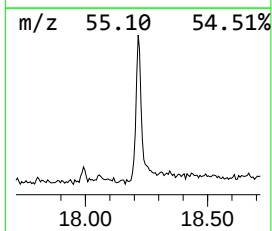
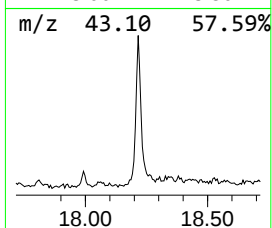
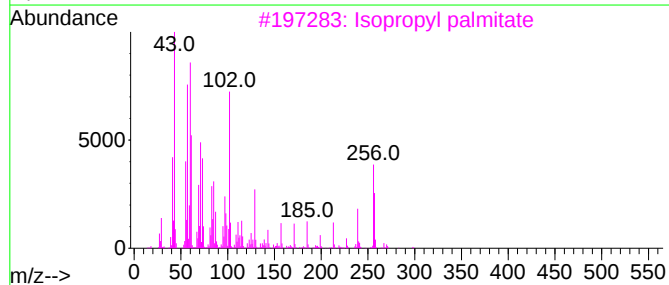
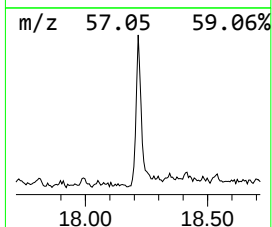
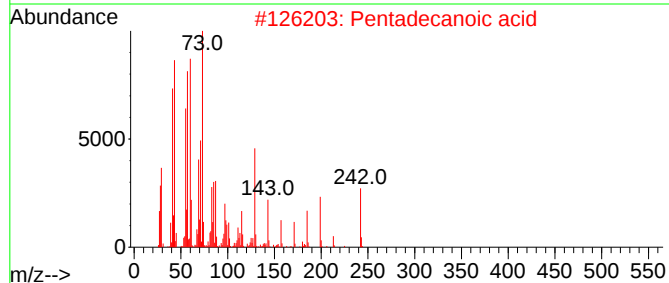
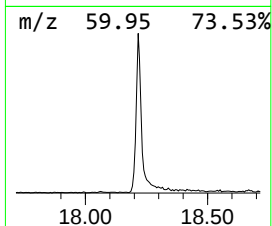
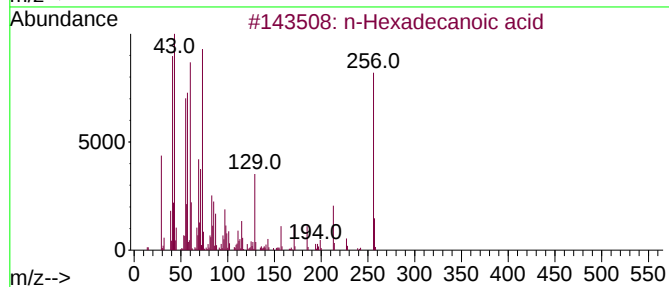
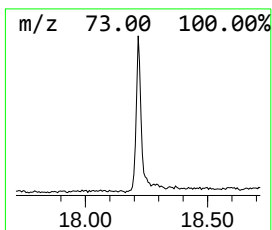
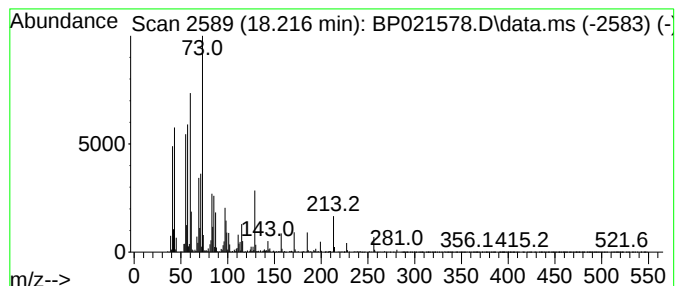
Instrument :
BNA_P
ClientSampleId :
921-J-SD-0.5-1.0-081524

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 6

R.T.	EstConc	Area	Relative to ISTD		R.T.	
18.216	2.94 ng	752908	Phenanthrene-d10		17.269	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid		242	C15H30O2	001002-84-2	74
3	Isopropyl palmitate		298	C19H38O2	000142-91-6	59
4	Tridecanoic acid		214	C13H26O2	000638-53-9	53
5	Dodecanoic acid		200	C12H24O2	000143-07-7	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP082024\
Data File : BP021578.D
Acq On : 20 Aug 2024 18:51
Operator : RC/JU
Sample : P3643-12
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
921-J-SD-0.5-1.0-081524

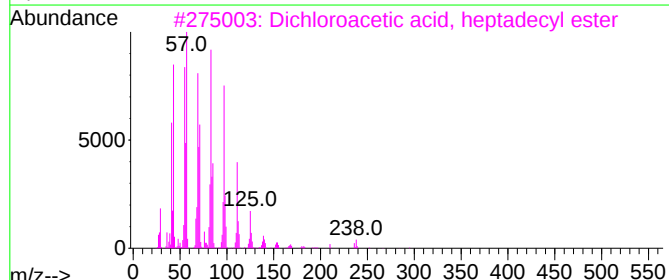
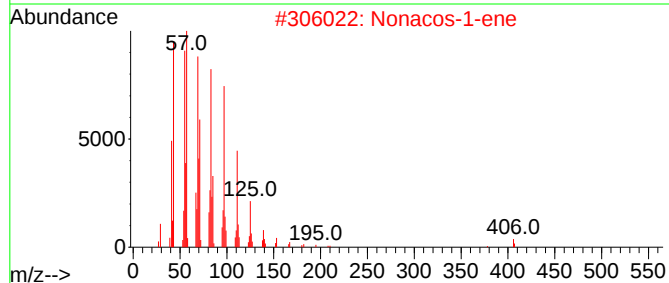
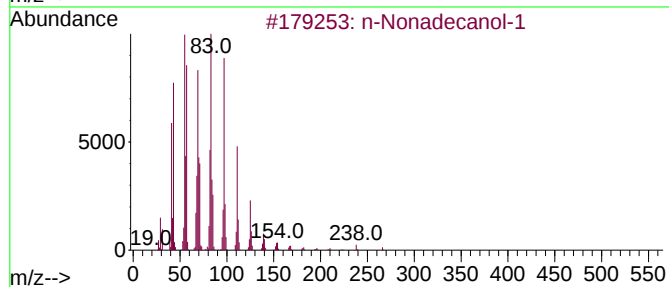
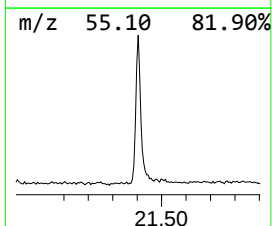
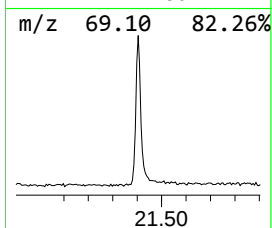
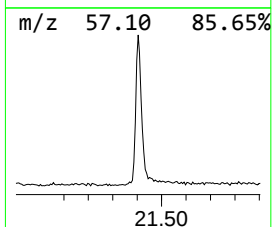
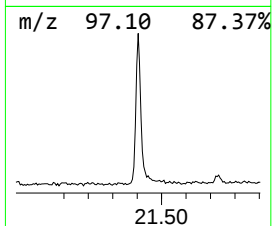
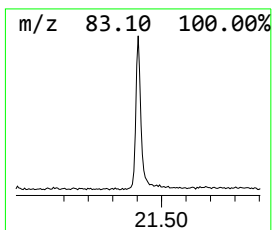
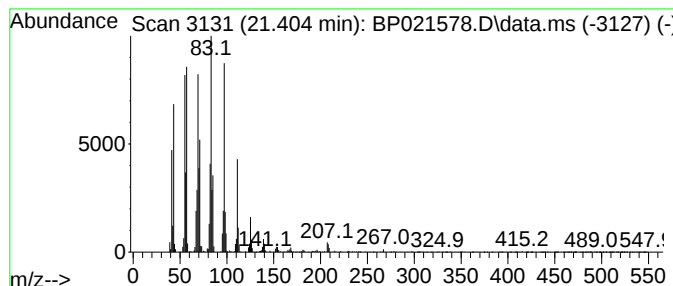
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 n-Nonadecanol-1 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.404	4.84 ng	1424690	Chrysene-d12	21.733

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Nonadecanol-1	284	C19H40O	001454-84-8	93
2			Nonacos-1-ene	406	C29H58	018835-35-3	91
3			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	91
4			Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	91
5			Behenic alcohol	326	C22H46O	000661-19-8	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP082024\
Data File : BP021578.D
Acq On : 20 Aug 2024 18:51
Operator : RC/JU
Sample : P3643-12
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
921-J-SD-0.5-1.0-081524

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	49.3	ng	4881300	1	7.804	1980450	20.0
Propylene Glycol	3.546	2.4	ng	241113	1	7.804	1980450	20.0
2-Pentanone, 4-...	4.934	3.6	ng	360292	1	7.804	1980450	20.0
1-Phenoxypropan...	11.334	3.4	ng	473152	2	10.593	2776900	20.0
unknown14.681	14.681	10.9	ng	2136930	3	14.457	3929070	20.0
n-Hexadecanoic ...	18.216	2.9	ng	752908	4	17.269	5130030	20.0
n-Nonadecanol-1	21.404	4.8	ng	1424690	5	21.733	5881370	20.0