

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061324\
 Data File : BP020619.D
 Acq On : 13 Jun 2024 20:19
 Operator : MA/JU
 Sample : P2864-05
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 WC-I

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-BP052924.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP020619.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.023	3	6	22	rVB	1734725	2620879	31.08%	4.556%
2	3.552	92	96	111	rBV	125999	185573	2.20%	0.323%
3	4.922	321	329	337	rVB2	176542	279417	3.31%	0.486%
4	5.370	398	405	418	rBV	2568734	3872345	45.91%	6.731%
5	6.928	662	670	691	rBV	2434501	4021297	47.68%	6.990%
6	7.746	801	809	816	rBV	885868	1377198	16.33%	2.394%
7	8.893	996	1004	1021	rBV	1598630	2608042	30.92%	4.534%
8	9.452	1092	1099	1107	rBV	73935	112902	1.34%	0.196%
9	10.299	1235	1243	1256	rBV2	89862	216545	2.57%	0.376%
10	10.522	1273	1281	1288	rBV	1195152	1915338	22.71%	3.329%
11	11.263	1398	1407	1424	rBV	120633	270994	3.21%	0.471%
12	12.987	1693	1700	1710	rBV	4607283	6196706	73.47%	10.772%
13	14.375	1925	1936	1943	rBV	1562372	2537440	30.09%	4.411%
14	14.598	1972	1974	1981	rVB	80792	94181	1.12%	0.164%
15	15.892	2186	2194	2214	rBV	3075396	4812854	57.07%	8.366%
16	17.181	2406	2413	2418	rBV	1941805	2977570	35.30%	5.176%
17	17.222	2418	2420	2427	rVV	124860	153326	1.82%	0.267%
18	17.316	2431	2436	2442	rVB	91850	155767	1.85%	0.271%
19	17.486	2458	2465	2475	rVB	102510	166891	1.98%	0.290%
20	18.134	2570	2575	2583	rBV2	655751	928723	11.01%	1.614%
21	18.286	2597	2601	2607	rVB3	51331	89559	1.06%	0.156%
22	19.316	2771	2776	2784	rBV	978088	1432952	16.99%	2.491%
23	19.457	2796	2800	2807	rBV3	217860	326024	3.87%	0.567%
24	19.692	2831	2840	2845	rBV	883783	1464103	17.36%	2.545%
25	19.916	2871	2878	2887	rVB	5175737	8433920	100.00%	14.661%
26	20.039	2893	2899	2908	rBV5	83098	270596	3.21%	0.470%
27	20.216	2924	2929	2932	rBV	189868	262559	3.11%	0.456%
28	20.316	2942	2946	2950	rVB	184596	242234	2.87%	0.421%
29	21.316	3112	3116	3134	rVB4	581595	1232624	14.62%	2.143%
30	21.633	3162	3170	3175	rBV2	2121452	4126015	48.92%	7.172%
31	21.675	3175	3177	3186	rVB	504341	802244	9.51%	1.395%
32	24.816	3706	3711	3712	rBV2	255322	406768	4.82%	0.707%
33	24.986	3732	3740	3750	rVB2	1034265	2933824	34.79%	5.100%

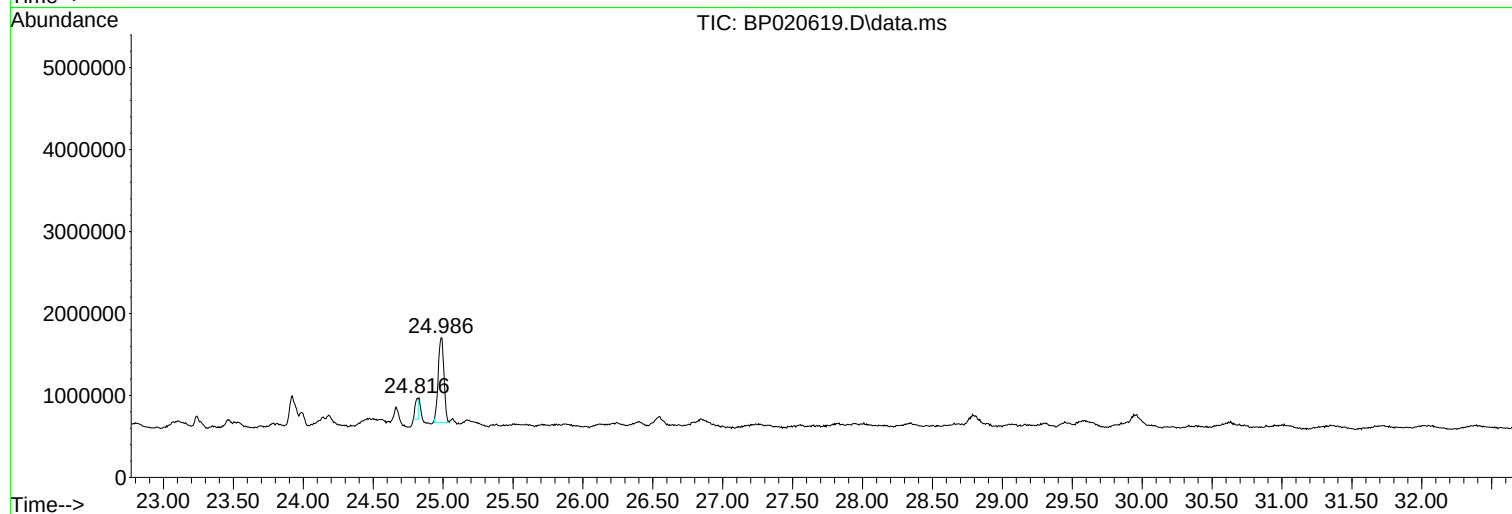
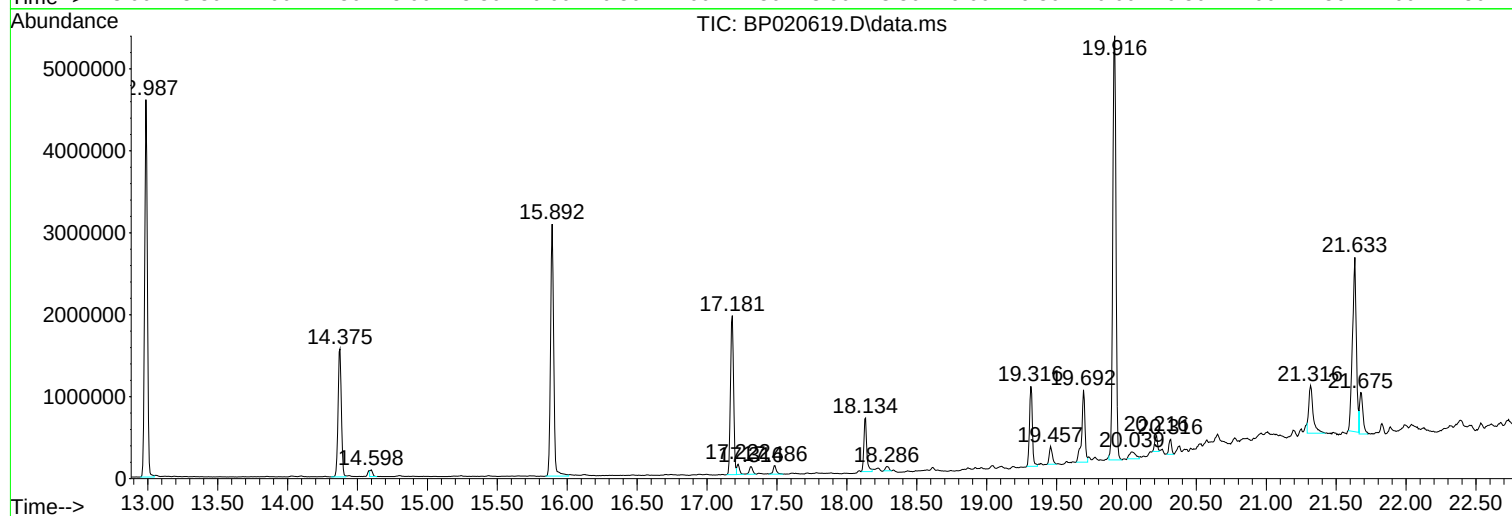
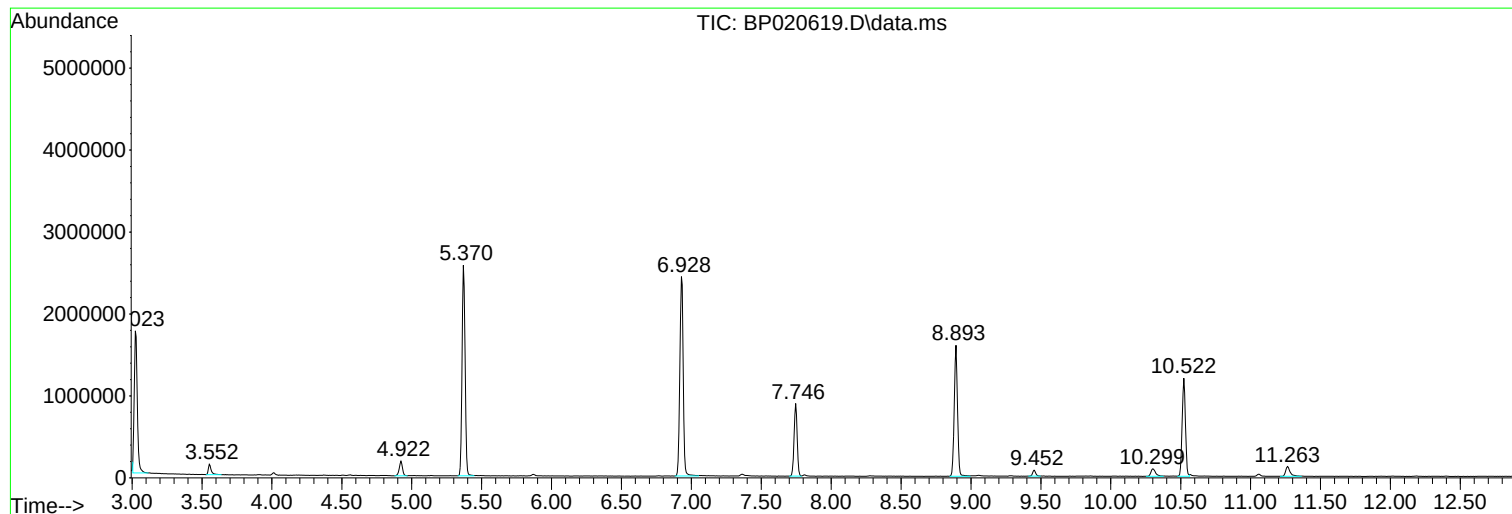
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP052924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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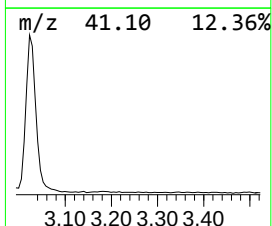
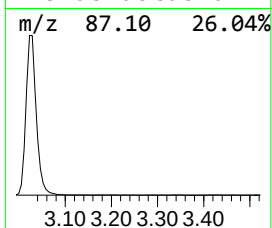
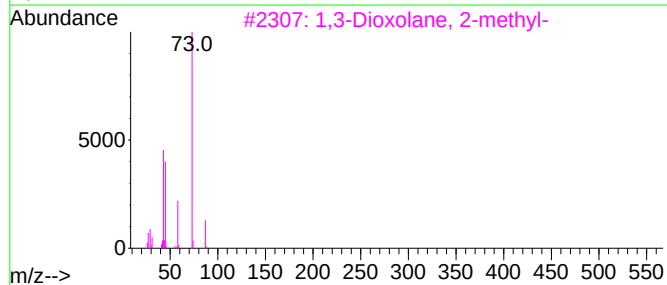
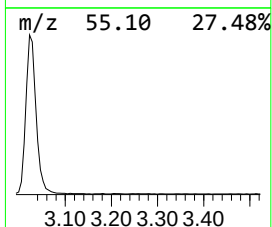
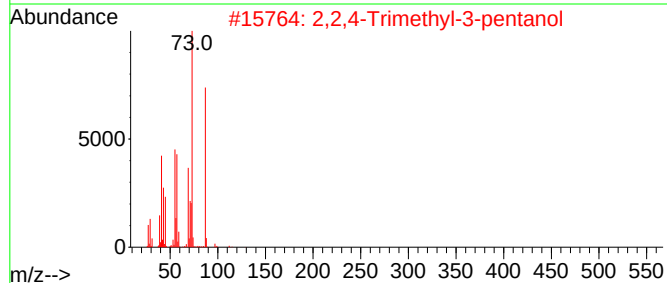
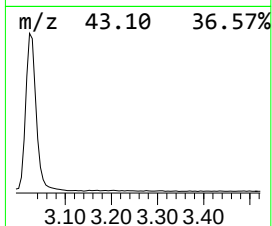
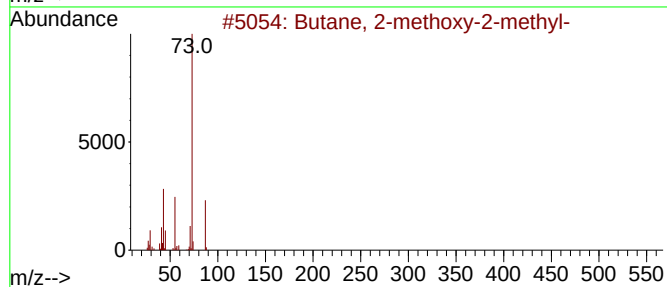
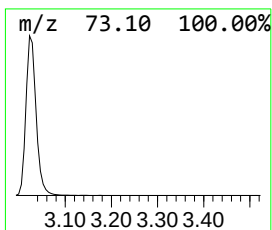
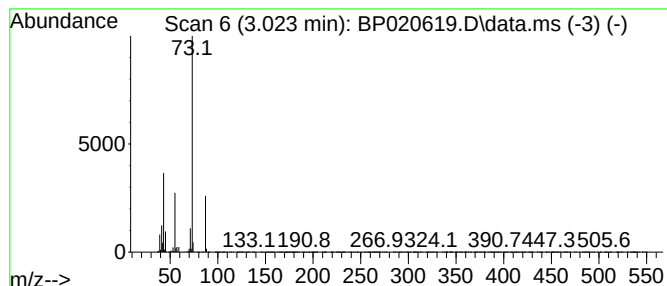
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
3.023	38.06 ng	2620880	1,4-Dichlorobenzene-d4	7.746

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	40
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17



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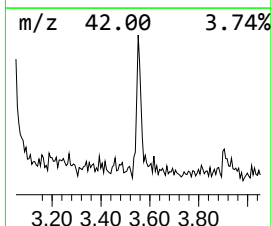
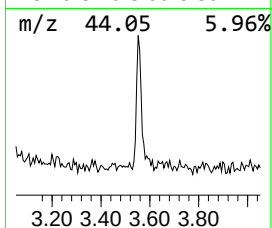
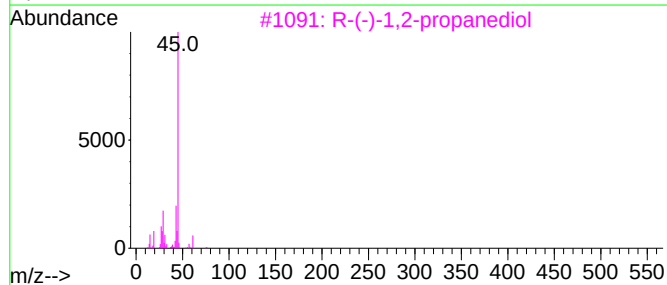
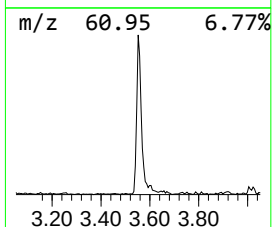
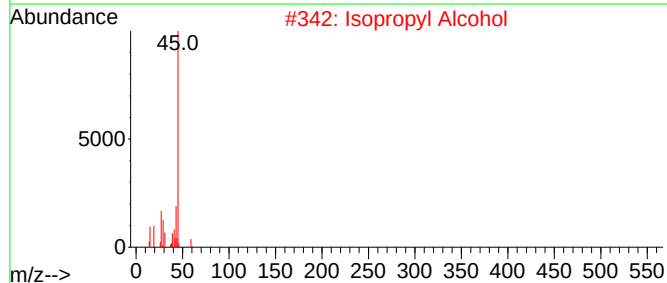
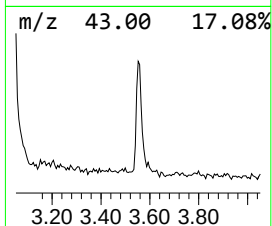
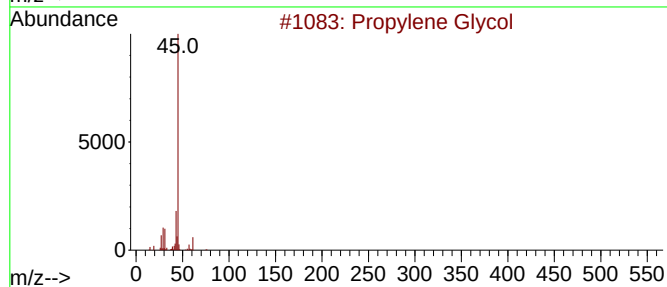
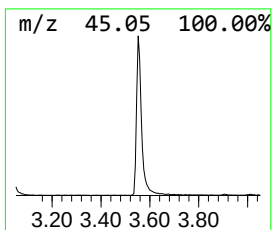
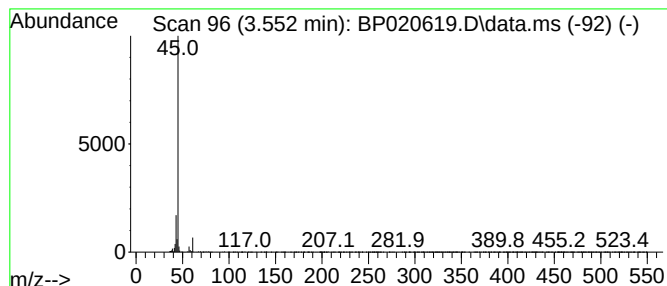
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Propylene Glycol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.552	2.69 ng	185573	1,4-Dichlorobenzene-d4	7.746

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propylene Glycol	76	C3H8O2	000057-55-6	74
2			Isopropyl Alcohol	60	C3H8O	000067-63-0	56
3			R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	43
4			(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	40
5			Hydrazine, (2-methoxyethyl)-	90	C3H10N2O	003044-15-3	9



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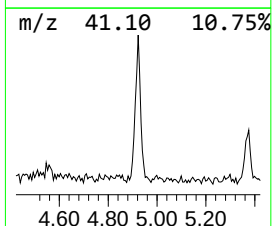
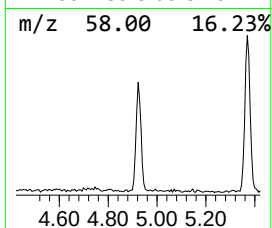
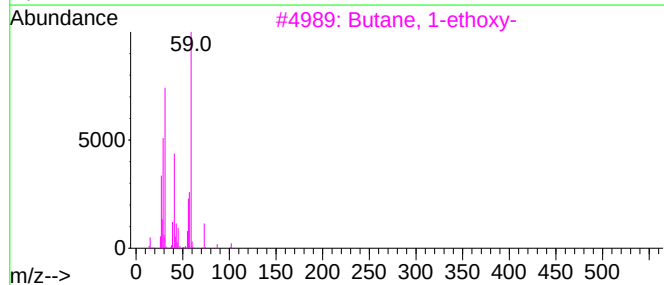
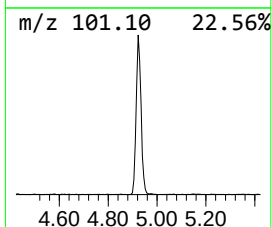
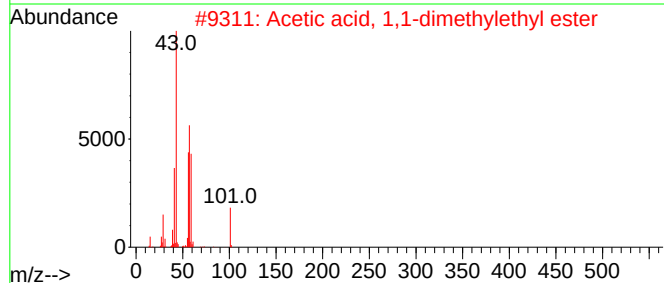
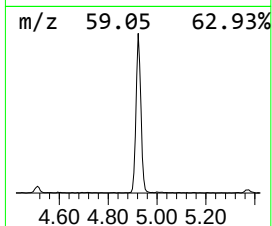
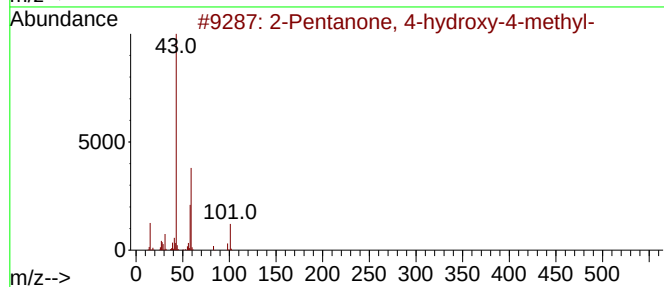
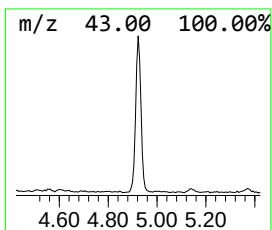
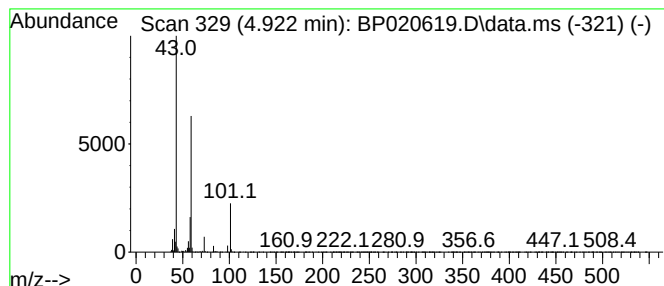
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.922	4.06 ng	279417	1,4-Dichlorobenzene-d4	7.746

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	17
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			Guanidine	59	CH5N3	000113-00-8	9



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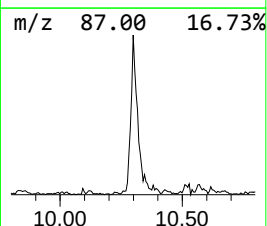
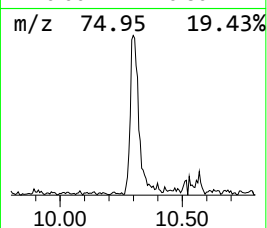
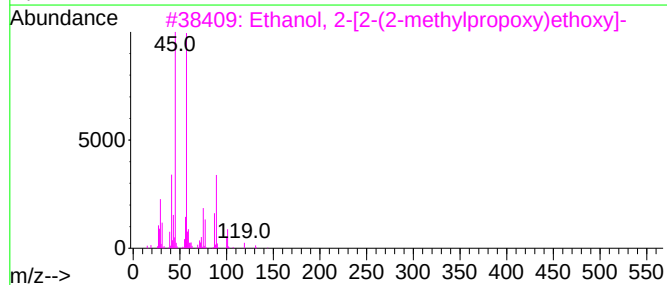
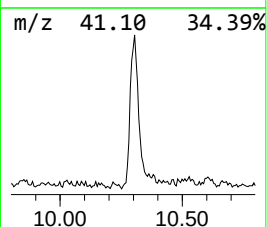
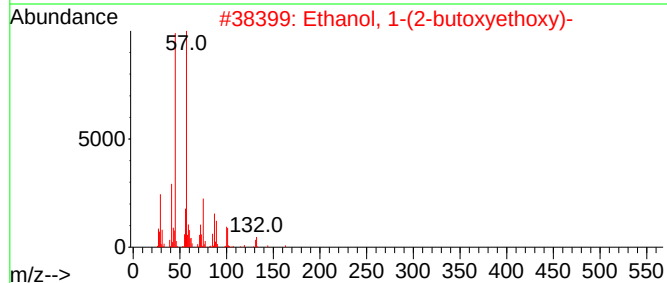
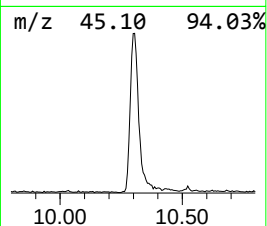
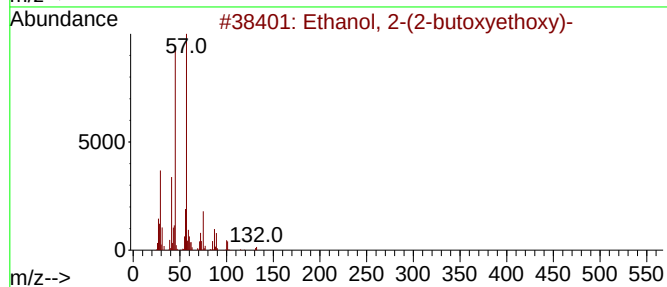
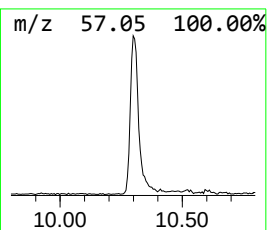
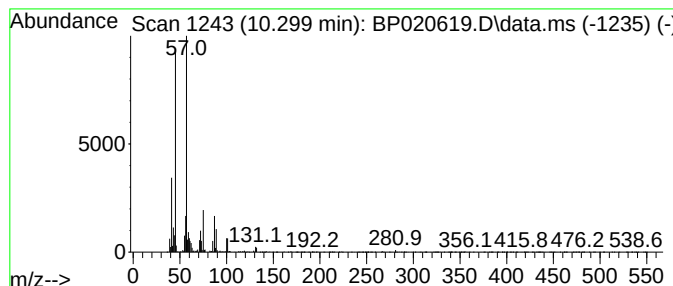
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.299	2.26 ng	216545	Naphthalene-d8	10.522

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			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	64
4			Acetaldehyde, di-sec-butyl acetal	174	C10H22O2	005314-41-0	50
5			Methoxyacetic acid, 2-butyl ester	146	C7H14O3	070159-90-9	47



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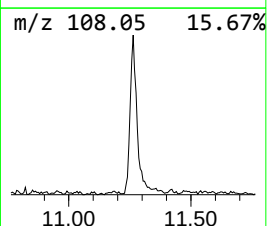
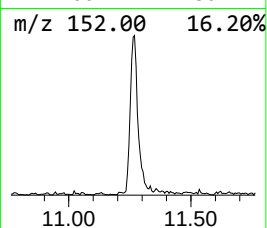
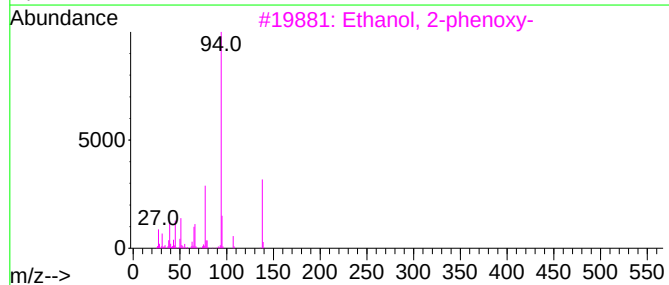
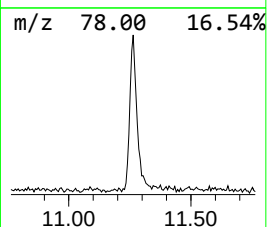
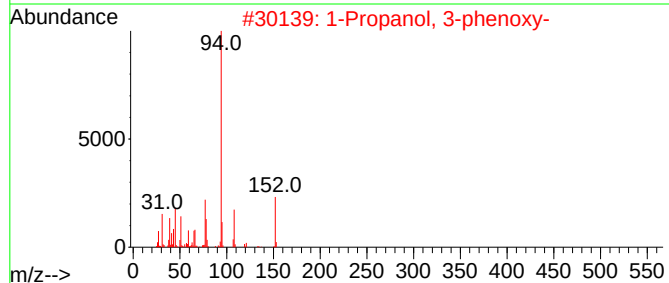
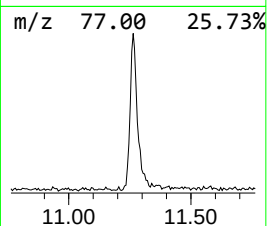
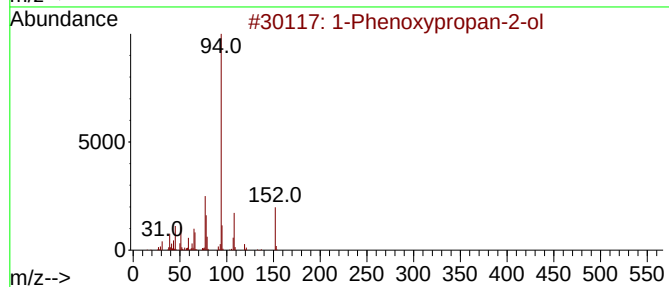
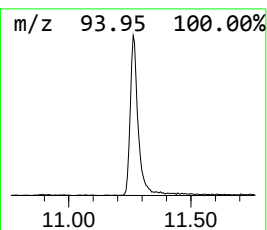
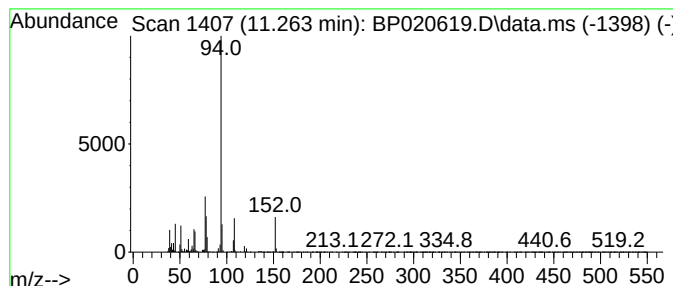
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Peak Number 5 1-Phenoxypropan-2-ol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.263	2.83 ng	270994	Naphthalene-d8	10.522

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	87
3			Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
4			1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	59
5			Carbonic acid, neopentyl phenyl ...	208	C12H16O3	013183-19-2	59



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WC-I

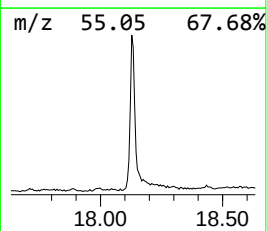
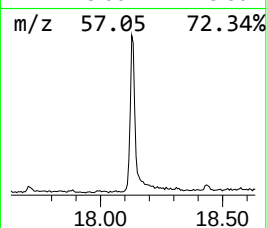
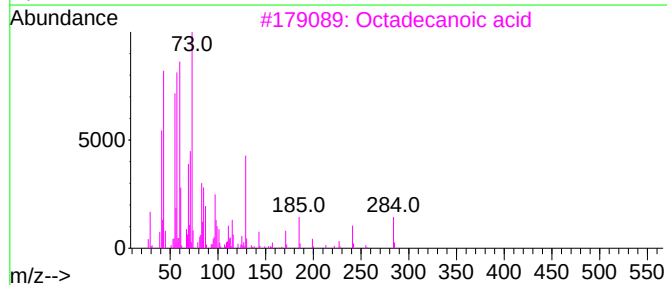
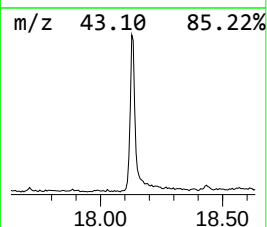
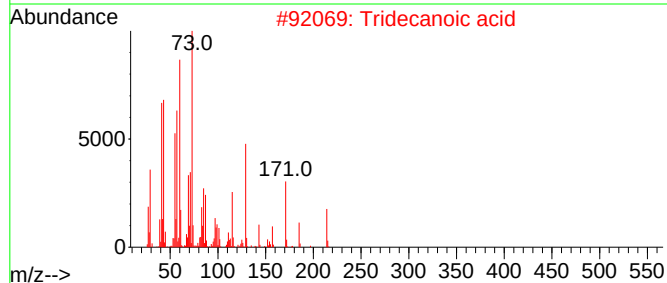
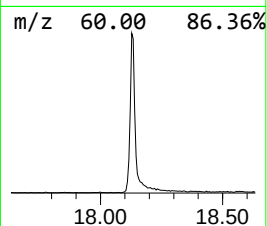
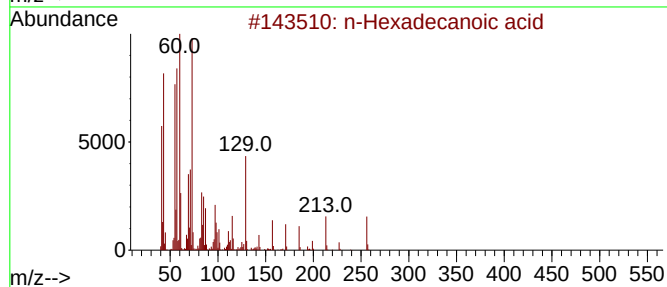
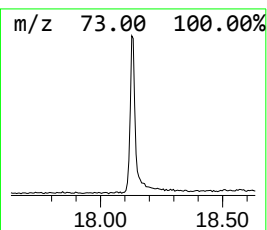
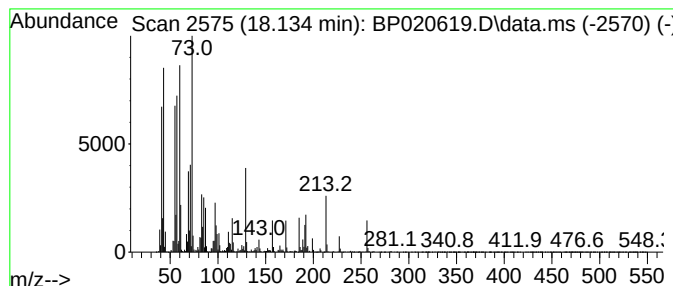
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.134	6.24 ng	928723	Phenanthrene-d10	17.181

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	95
3			Octadecanoic acid	284	C18H36O2	000057-11-4	93
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
5			n-Decanoic acid	172	C10H20O2	000334-48-5	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061324\
Data File : BP020619.D
Acq On : 13 Jun 2024 20:19
Operator : MA/JU
Sample : P2864-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
WC-I

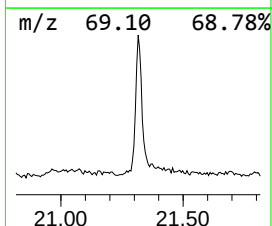
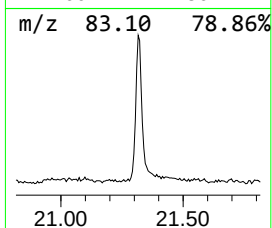
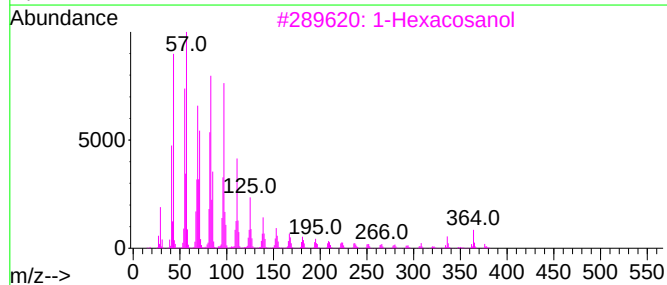
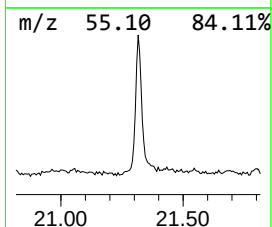
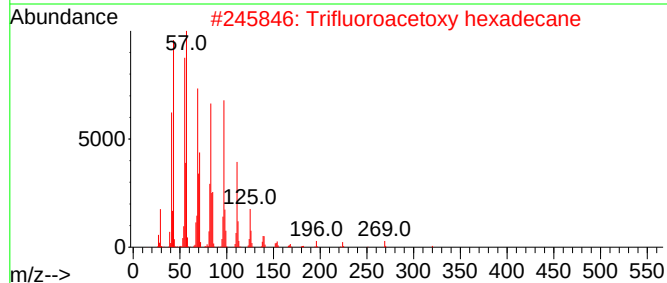
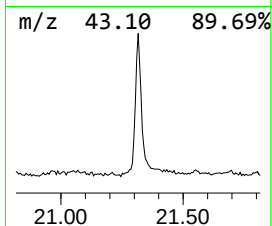
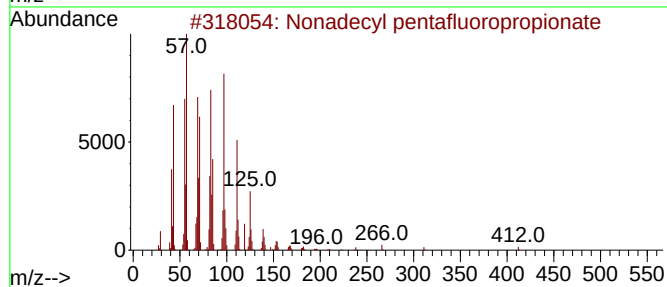
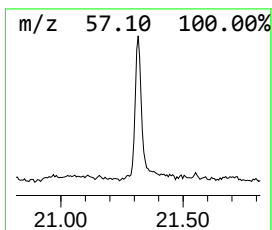
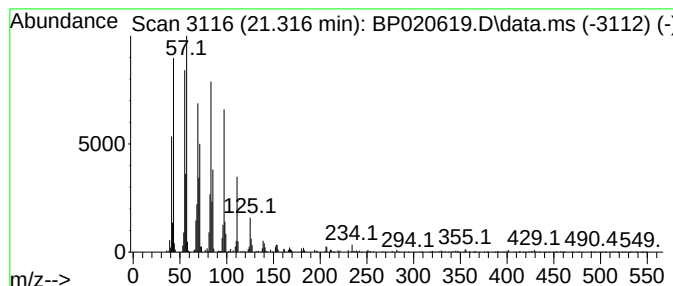
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Nonadecyl pentafluoropropio... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.316	5.97 ng	1232620	Chrysene-d12	21.633

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
2			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
3			1-Hexacosanol	382	C26H54O	000506-52-5	91
4			Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91
5			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061324\
Data File : BP020619.D
Acq On : 13 Jun 2024 20:19
Operator : MA/JU
Sample : P2864-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
WC-I

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP052924.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...	3.023	38.1	ng	2620880	1	7.746	1377200	20.0
Propylene Glycol	3.552	2.7	ng	185573	1	7.746	1377200	20.0
2-Pentanone, 4-...	4.922	4.1	ng	279417	1	7.746	1377200	20.0
Ethanol, 2-(2-b...	10.299	2.3	ng	216545	2	10.522	1915340	20.0
1-Phenoxypropan...	11.263	2.8	ng	270994	2	10.522	1915340	20.0
n-Hexadecanoic ...	18.134	6.2	ng	928723	4	17.181	2977570	20.0
Nonadecyl penta...	21.316	6.0	ng	1232620	5	21.633	4126020	20.0