

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP081524\
 Data File : BP021520.D
 Acq On : 15 Aug 2024 19:20
 Operator : RC/JU
 Sample : P3582-04
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 S-855-J-SO-3-3.5-081224

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: BP021520.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	26	rVB	2975778	4621370	34.99%	5.194%
2	3.546	90	95	102	rBV	262473	357700	2.71%	0.402%
3	4.934	325	331	338	rVB	208608	304585	2.31%	0.342%
4	5.393	402	409	420	rBV	4438933	6676456	50.55%	7.503%
5	6.957	667	675	686	rBV	4245113	6961094	52.70%	7.823%
6	7.805	811	819	825	rBV	1559562	2549109	19.30%	2.865%
7	8.946	1004	1013	1025	rBV	2425253	4267585	32.31%	4.796%
8	9.504	1102	1108	1115	rBV	86054	133567	1.01%	0.150%
9	10.593	1283	1293	1300	rBV	2098893	3484550	26.38%	3.916%
10	11.322	1410	1417	1427	rBV	296618	553617	4.19%	0.622%
11	13.051	1704	1711	1722	rBV	5967850	8970461	67.91%	10.081%
12	14.439	1938	1947	1953	rBV	3057962	4626055	35.02%	5.199%
13	14.675	1984	1987	1992	rVB	125085	168835	1.28%	0.190%
14	15.945	2191	2203	2211	rBV	4692680	6890190	52.16%	7.744%
15	17.228	2415	2421	2426	rBV	3592666	5514515	41.75%	6.197%
16	17.275	2426	2429	2435	rVB	223137	319811	2.42%	0.359%
17	17.363	2437	2444	2450	rVB	96680	166385	1.26%	0.187%
18	18.175	2571	2582	2591	rBV2	520616	1028726	7.79%	1.156%
19	19.351	2777	2782	2790	rBV	932815	1253751	9.49%	1.409%
20	19.504	2803	2808	2818	rBV2	355769	619690	4.69%	0.696%
21	19.727	2837	2846	2854	rBV	699286	1273814	9.64%	1.432%
22	19.951	2876	2884	2895	rVB	9230860	13208803	100.00%	14.845%
23	20.245	2931	2934	2942	rVB	129229	197002	1.49%	0.221%
24	21.363	3120	3124	3131	rVB4	367463	574912	4.35%	0.646%
25	21.621	3164	3168	3171	rBV	296508	468660	3.55%	0.527%
26	21.680	3171	3178	3183	rVV2	3888622	6762103	51.19%	7.600%
27	21.721	3183	3185	3196	rVB	433980	640395	4.85%	0.720%
28	23.910	3551	3557	3564	rVB	416926	822999	6.23%	0.925%
29	23.998	3566	3572	3579	rBV	195835	576709	4.37%	0.648%
30	25.086	3746	3757	3768	rBV	1748596	4986261	37.75%	5.604%

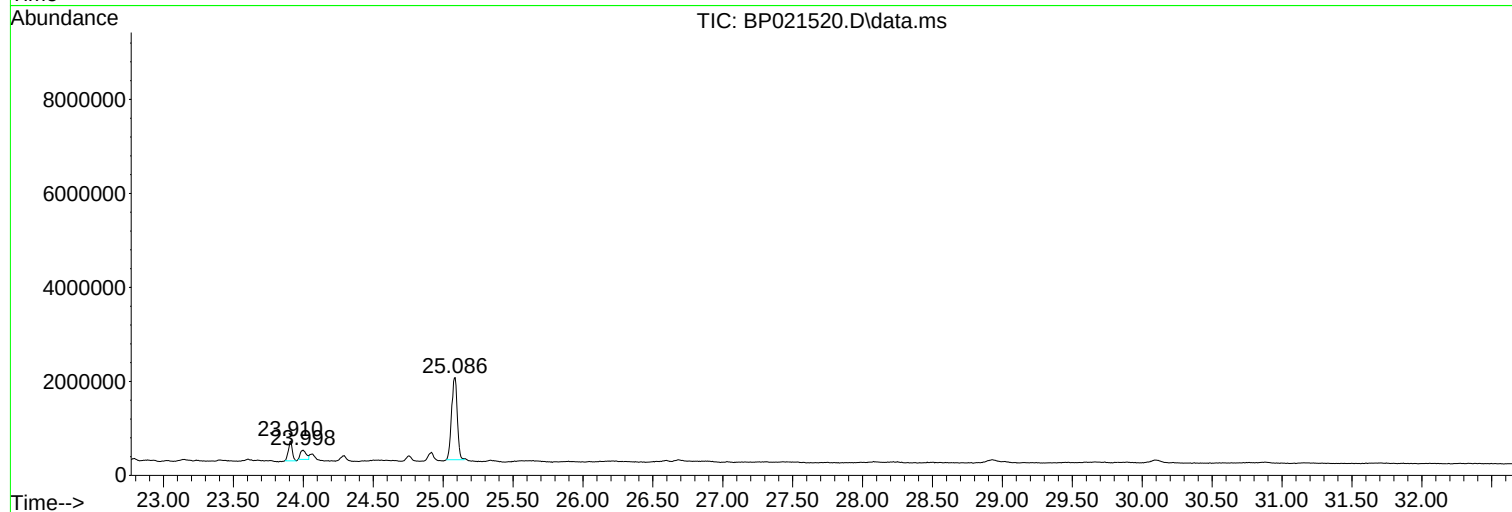
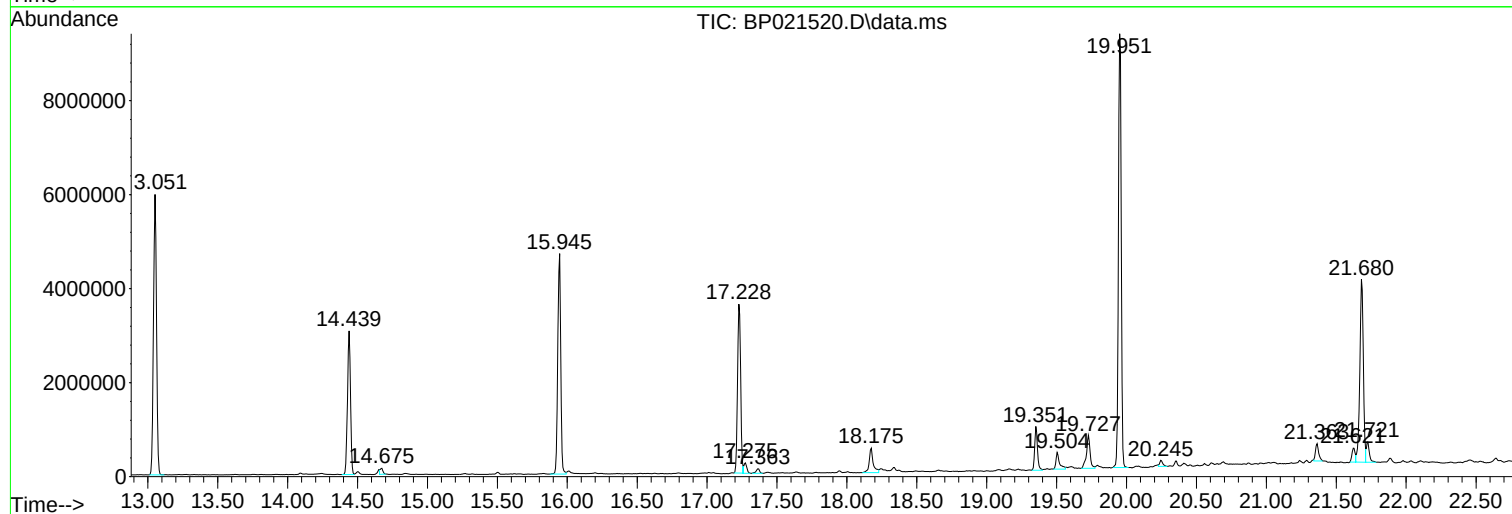
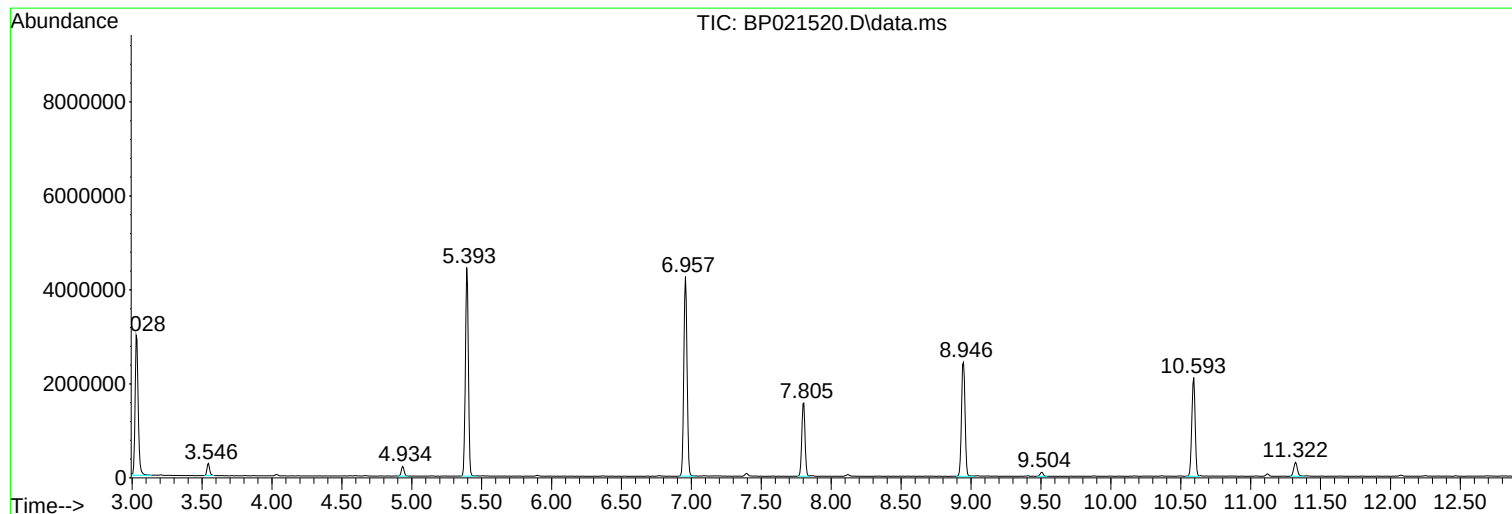
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP081324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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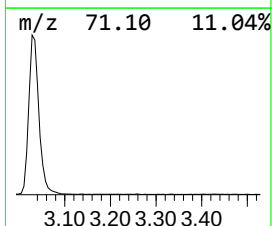
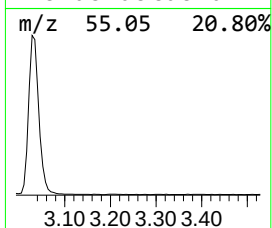
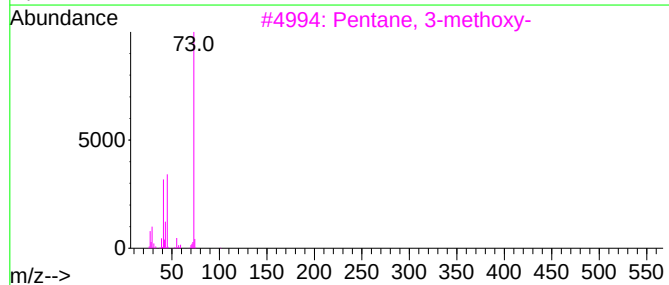
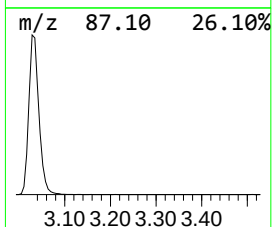
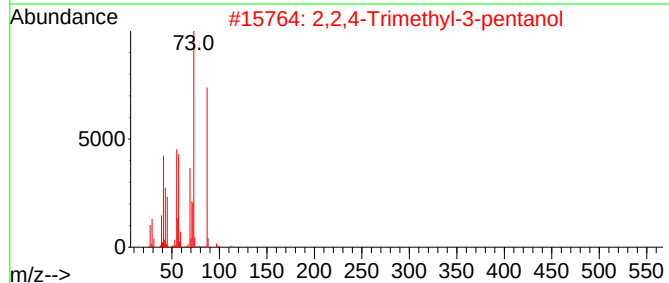
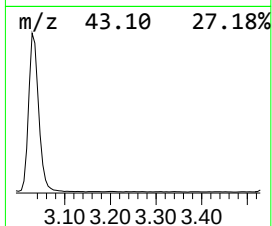
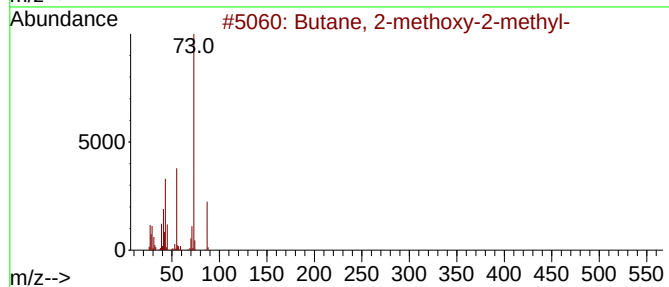
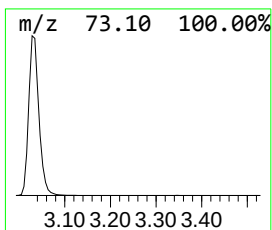
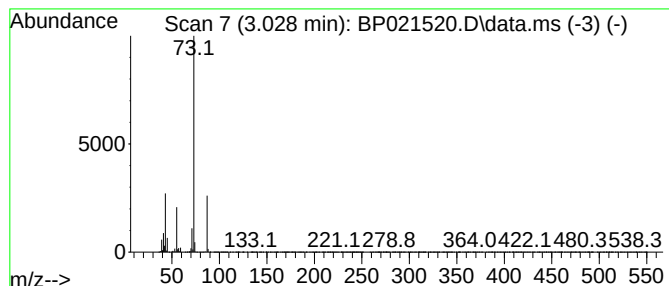
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	36.26 ng	4621370	1,4-Dichlorobenzene-d4	7.805

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			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
5			N-Ethylformamide	73	C3H7NO	000627-45-2	9



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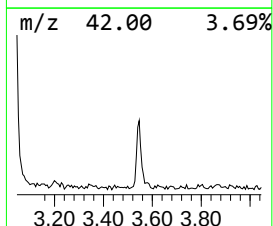
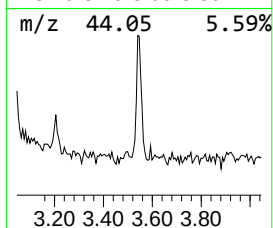
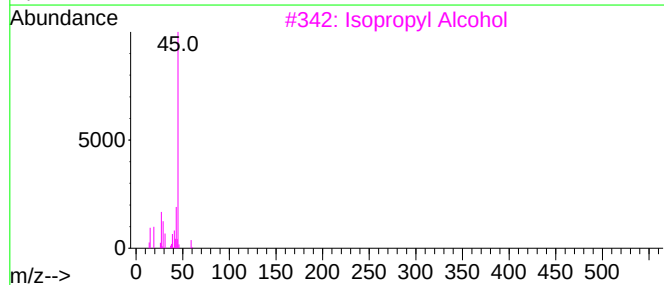
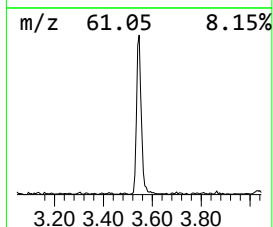
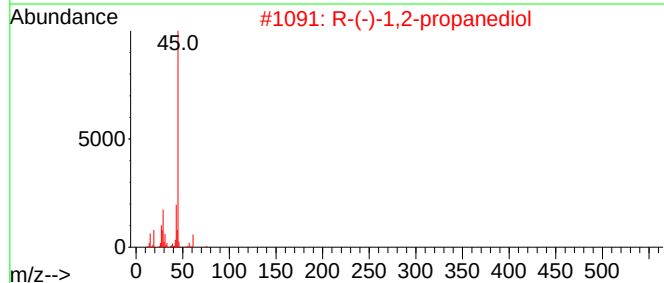
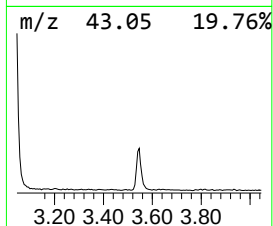
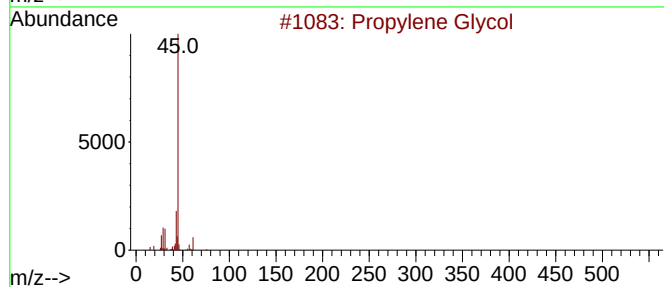
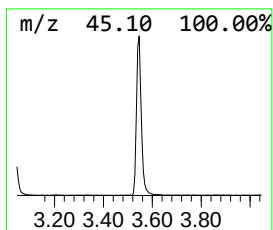
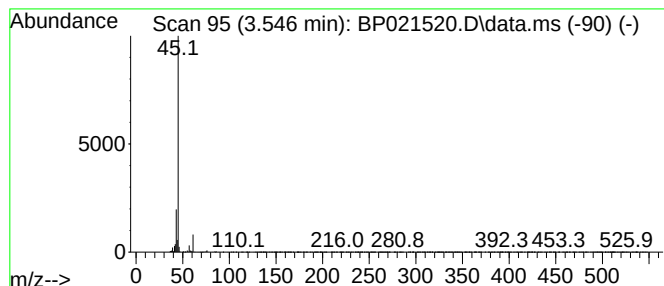
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Propylene Glycol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.546	2.81 ng	357700	1,4-Dichlorobenzene-d4	7.805

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		Isopropyl Alcohol	60	C3H8O	000067-63-0	56
4		(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	37
5		2-Heptanol	116	C7H16O	000543-49-7	9



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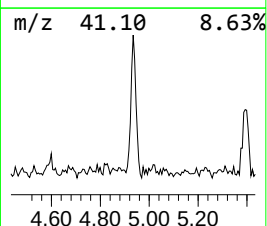
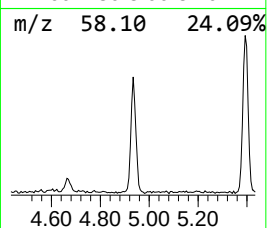
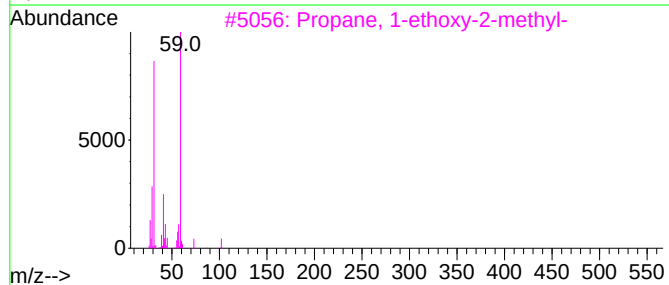
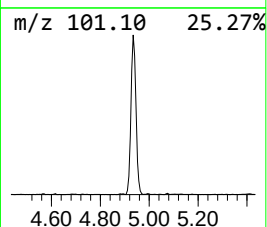
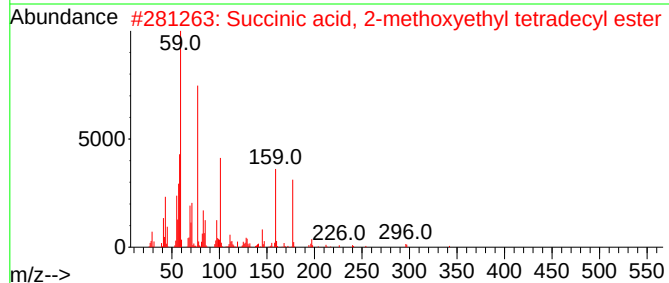
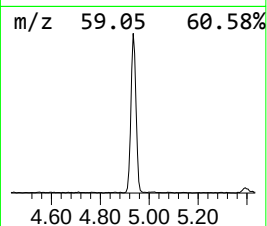
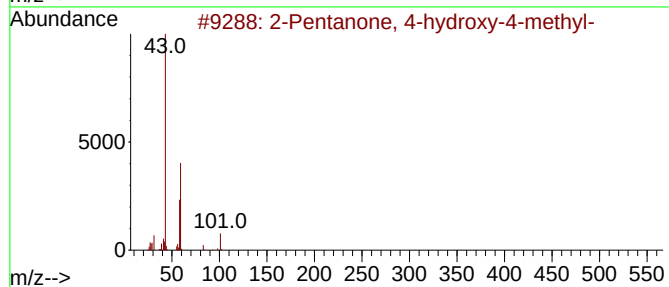
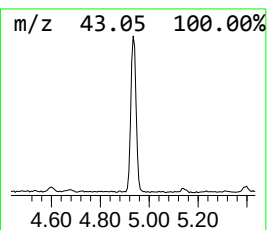
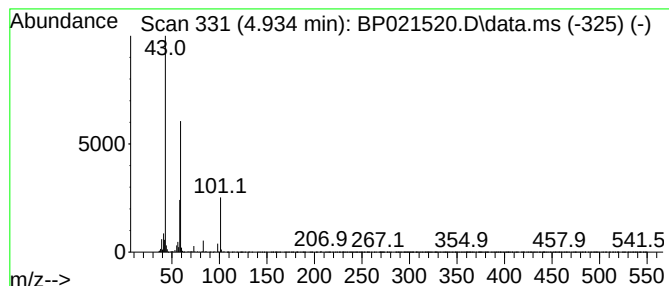
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.934	2.39 ng	304585	1,4-Dichlorobenzene-d4	7.805

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	78
2			Succinic acid, 2-methoxyethyl te...	372	C21H40O5	1000325-81-3	36
3			Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	16
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	12
5			2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	12



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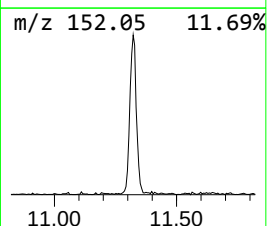
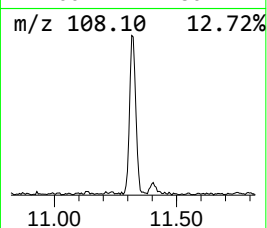
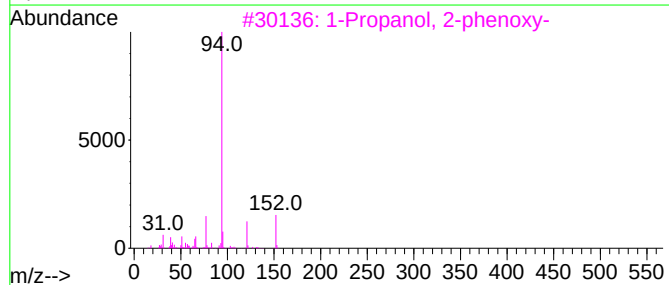
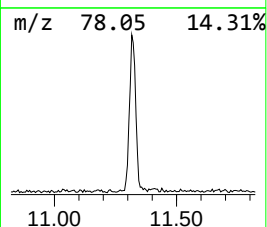
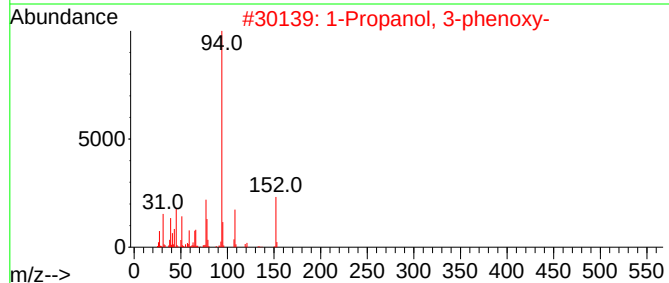
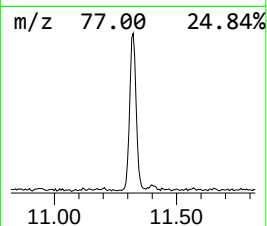
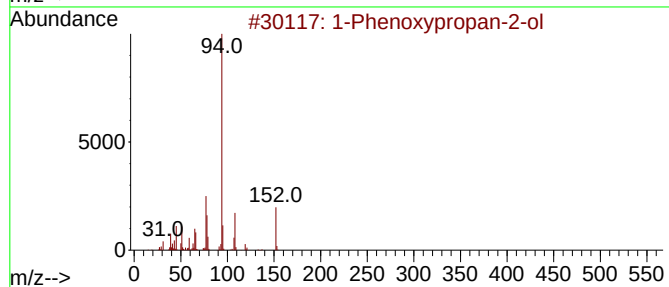
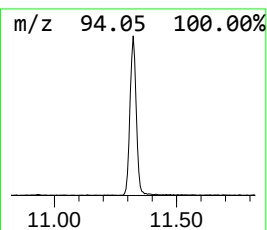
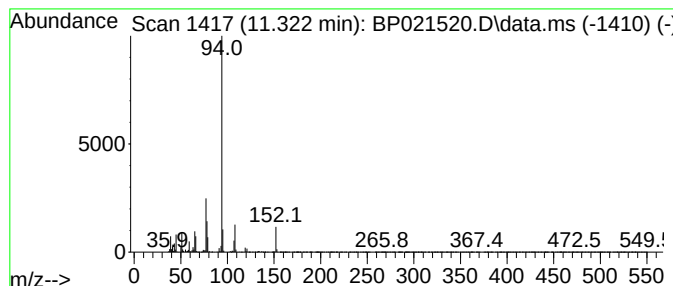
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Peak Number 4 1-Phenoxypropan-2-ol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.322	3.18 ng	553617	Naphthalene-d8	10.593

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	95
2			1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	87
3			1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	64
4			Carbonic acid, neopentyl phenyl ...	208	C12H16O3	013183-19-2	64
5			Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64



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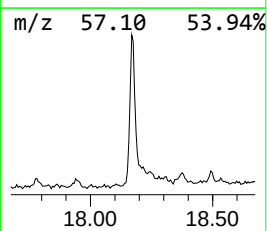
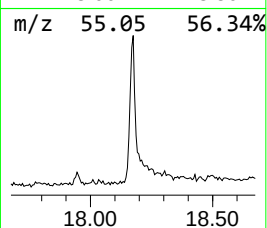
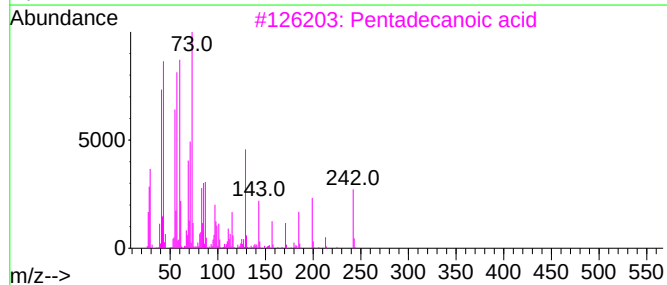
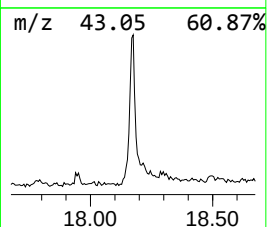
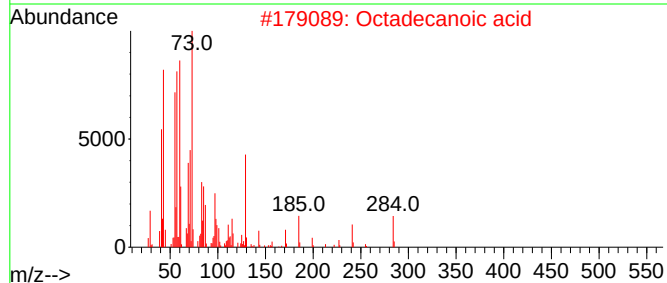
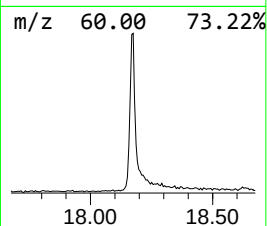
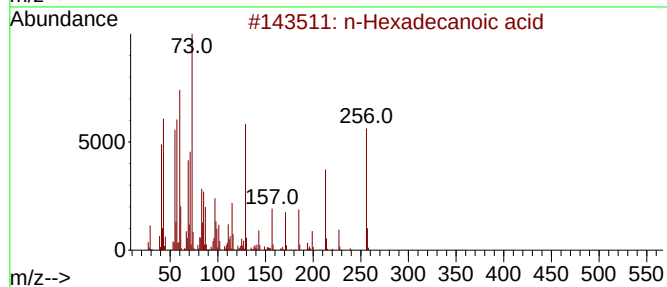
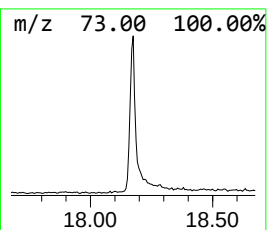
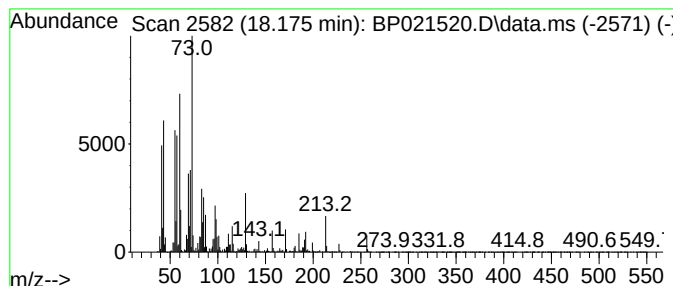
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.175	3.73 ng	1028730	Phenanthrene-d10	17.227

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2			Octadecanoic acid	284	C18H36O2	000057-11-4	74
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	64
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	59
5			Tridecanoic acid	214	C13H26O2	000638-53-9	59



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S-855-J-SO-3-3.5-081224

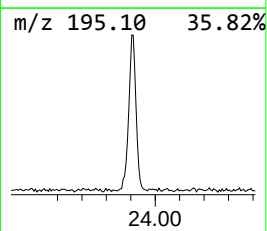
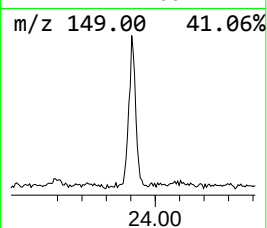
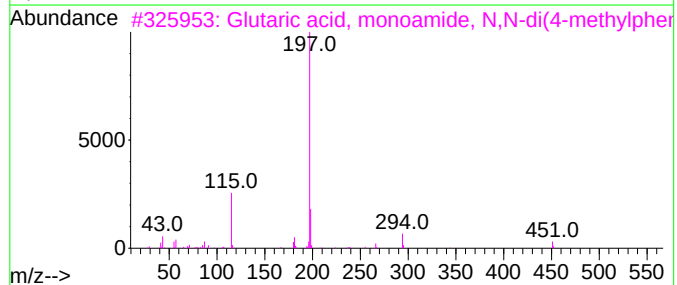
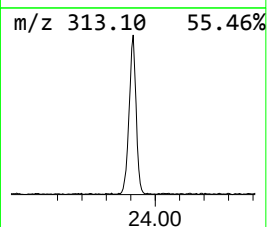
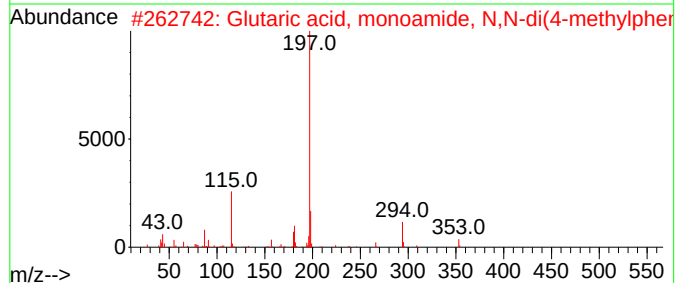
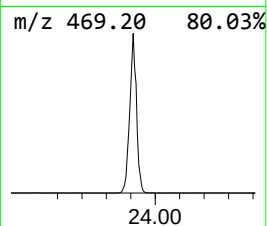
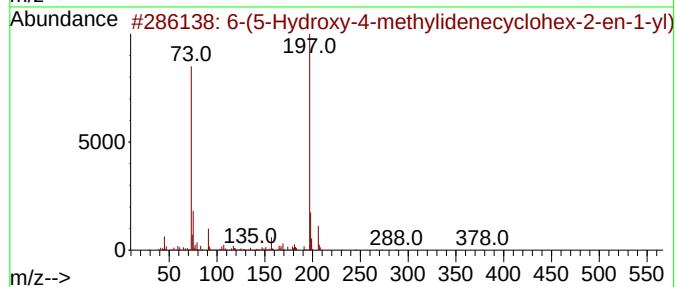
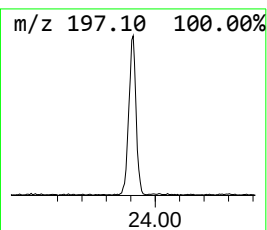
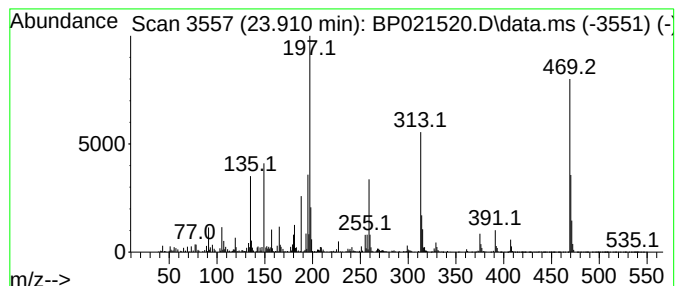
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown23.910 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.910	3.30 ng	822999	Perylene-d12	25.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	6-(5-Hydroxy-4-methylidenecyclohex-2-en-1-yl)	378	C21H38O2Si2	1000495-91-4	18		
2	Glutaric acid, monoamide, N,N-di(4-methylphenyl)	353	C22H27NO3	1000360-23-0	14		
3	Glutaric acid, monoamide, N,N-di(4-methylphenyl)	451	C29H41NO3	1000360-23-9	14		
4	13-Methyl-9-oxo-2-oxa-4,10-diazabicyclo[3.3.1]non-5-ene	305	C13H11N3O4S	1000410-02-0	14		
5	1'H-Cholesta-2,4,6-trieno[3,2-b]pyrene	469	C34H47N	038389-25-2	14		



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP081524\
Data File : BP021520.D
Acq On : 15 Aug 2024 19:20
Operator : RC/JU
Sample : P3582-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
S-855-J-SO-3-3.5-081224

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	36.3	ng	4621370	1	7.805	2549110	20.0
Propylene Glycol	3.546	2.8	ng	357700	1	7.805	2549110	20.0
2-Pentanone, 4-...	4.934	2.4	ng	304585	1	7.805	2549110	20.0
1-Phenoxypropan...	11.322	3.2	ng	553617	2	10.593	3484550	20.0
n-Hexadecanoic ...	18.175	3.7	ng	1028730	4	17.227	5514520	20.0
unknown23.910	23.910	3.3	ng	822999	6	25.086	4986260	20.0