

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP060524\
 Data File : BP020527.D
 Acq On : 05 Jun 2024 22:00
 Operator : MA/JU
 Sample : P2662-01
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 WCS-TPR

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: BP020527.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.040	4	9	26	rVB	2925431	3643074	21.67%	4.514%
2	3.558	93	97	110	rBV	498473	654489	3.89%	0.811%
3	5.381	399	407	416	rBV	5184740	7664454	45.58%	9.496%
4	6.934	661	671	690	rBV	5131256	7931846	47.17%	9.827%
5	7.363	739	744	755	rBV	132806	212960	1.27%	0.264%
6	7.769	804	813	820	rBV	865084	1444522	8.59%	1.790%
7	8.910	996	1007	1018	rBV	3094418	5252237	31.24%	6.507%
8	9.469	1093	1102	1108	rBV	110176	179316	1.07%	0.222%
9	10.528	1275	1282	1290	rBV	1084863	1981714	11.79%	2.455%
10	11.275	1400	1409	1418	rBV	281353	509469	3.03%	0.631%
11	13.004	1694	1703	1711	rBV	7246963	11608128	69.03%	14.382%
12	14.392	1931	1939	1946	rBV	1704916	2558847	15.22%	3.170%
13	15.904	2189	2196	2205	rBV	5928960	8630180	51.32%	10.692%
14	17.198	2409	2416	2430	rBV	1999853	3035735	18.05%	3.761%
15	18.145	2572	2577	2589	rBV2	317522	539879	3.21%	0.669%
16	19.480	2800	2804	2821	rVB	154566	237120	1.41%	0.294%
17	19.933	2875	2881	2887	rBV	13447444	16815089	100.00%	20.833%
18	21.333	3114	3119	3126	rBV	416419	750973	4.47%	0.930%
19	21.645	3167	3172	3180	rVB2	2236491	3387590	20.15%	4.197%
20	24.992	3732	3741	3753	rVB	1330226	3676959	21.87%	4.556%

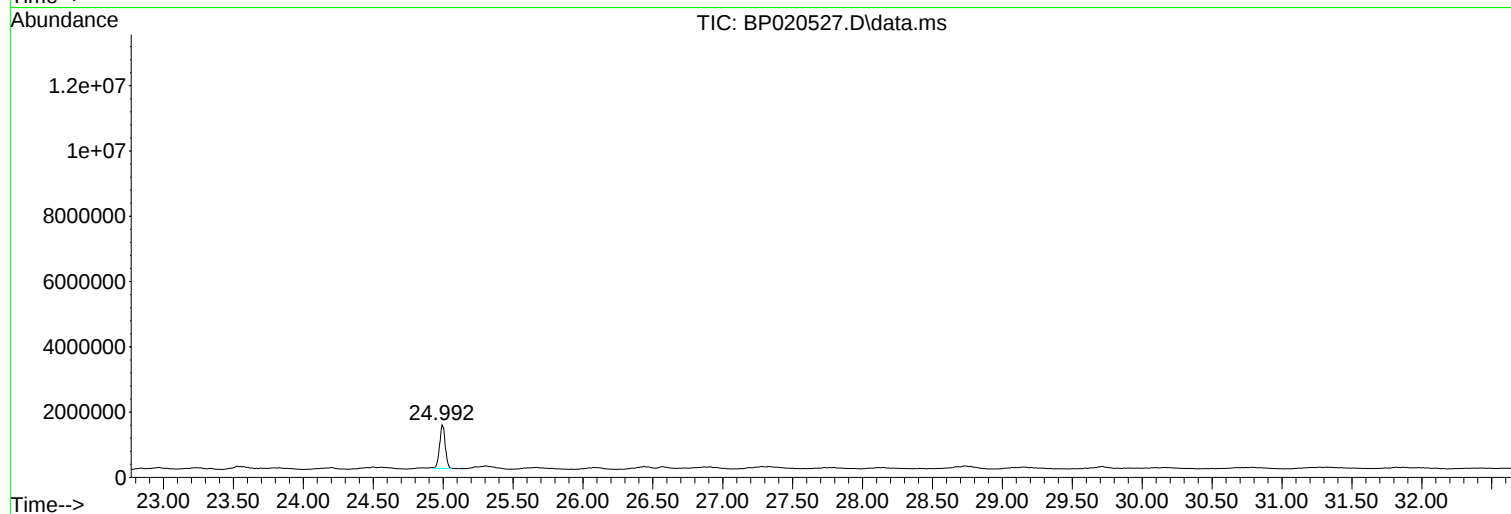
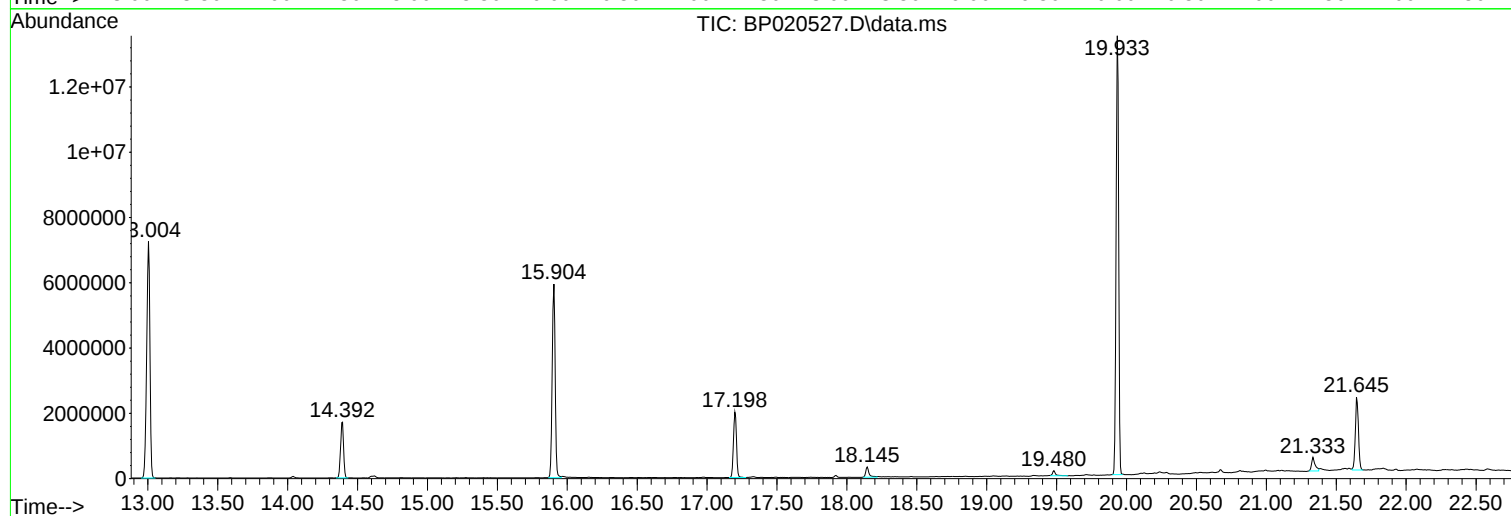
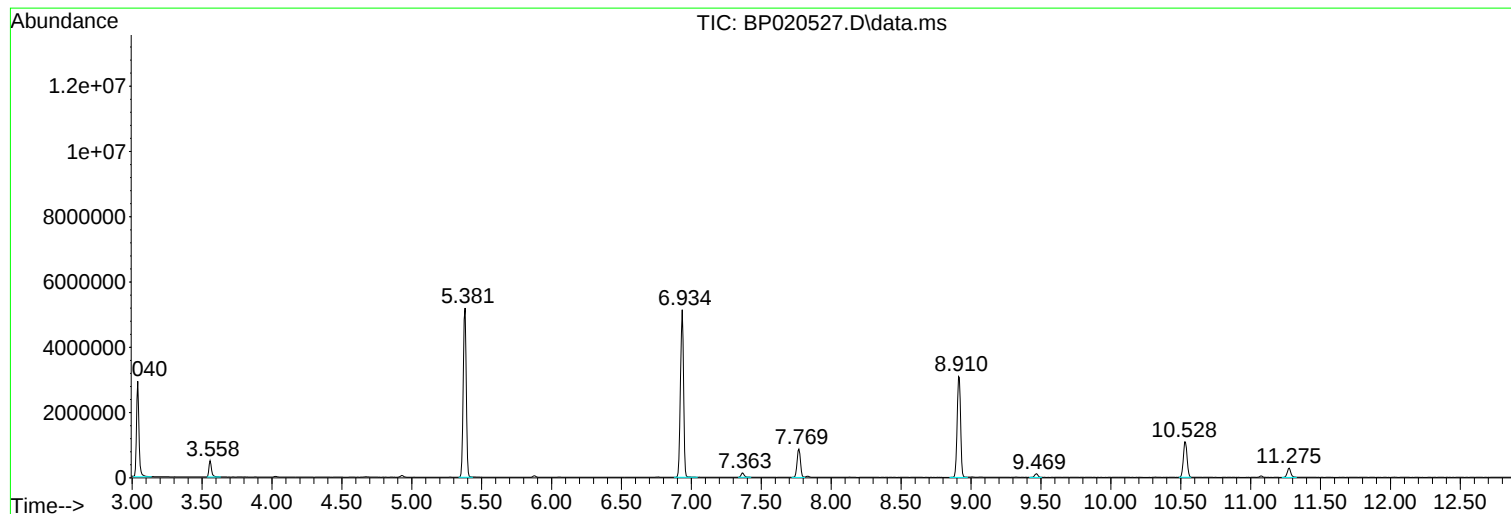
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP052924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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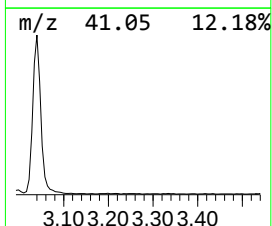
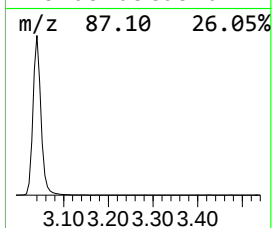
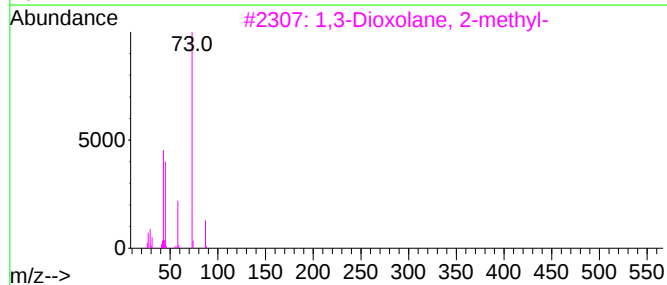
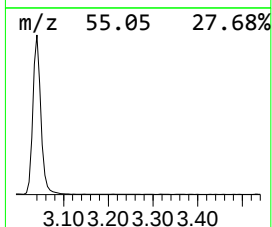
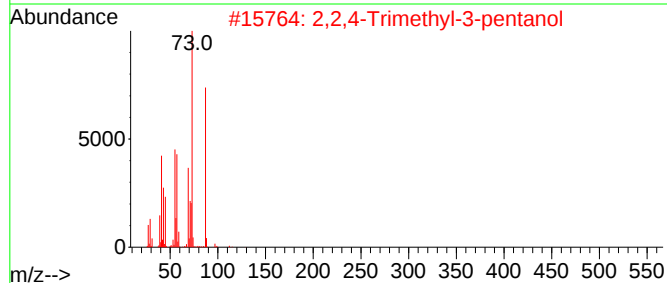
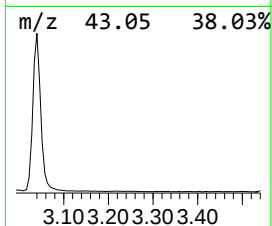
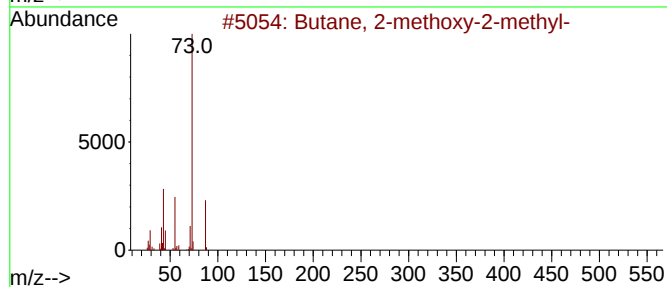
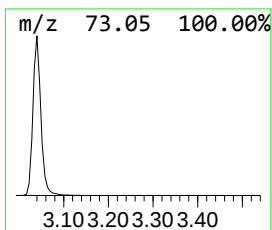
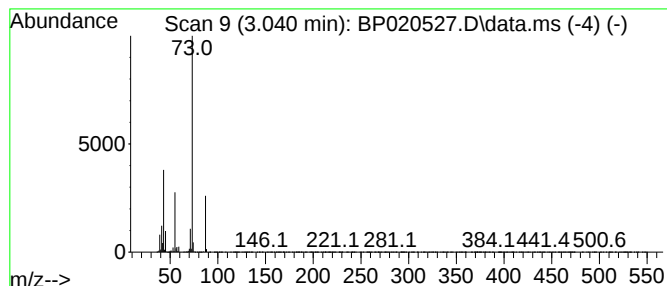
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
3.040	50.44 ng	3643070	1,4-Dichlorobenzene-d4	7.769

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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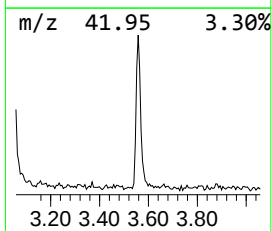
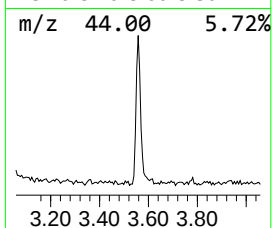
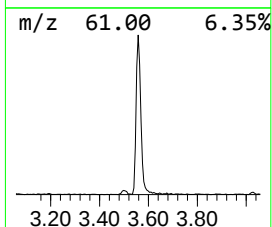
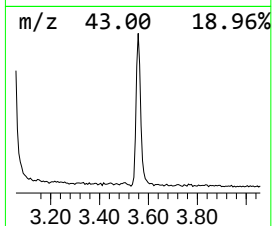
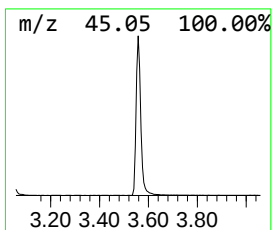
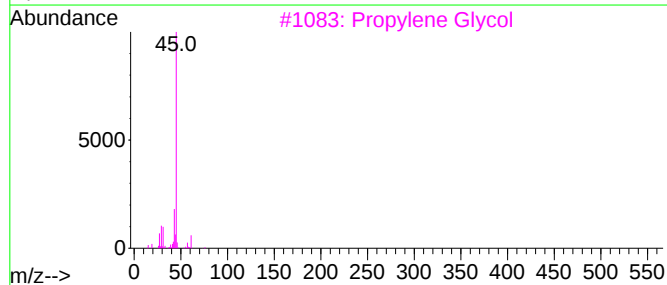
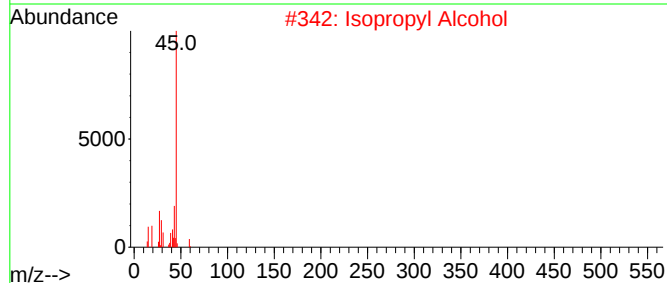
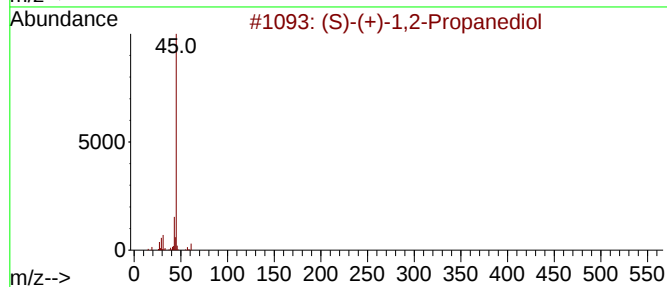
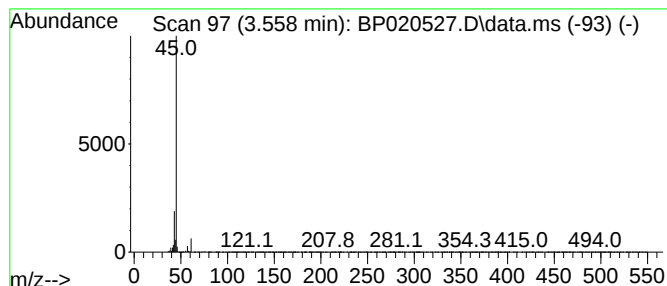
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 (S)-(+)-1,2-Propanediol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.558	9.06 ng	654489	1,4-Dichlorobenzene-d4	7.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-1,2-Propanediol			76	C3H8O2	004254-15-3	64
2	Isopropyl Alcohol			60	C3H8O	000067-63-0	56
3	Propylene Glycol			76	C3H8O2	000057-55-6	43
4	R-(-)-1,2-propanediol			76	C3H8O2	004254-14-2	43
5	Propanoic acid, 2-hydroxy-, meth...			104	C4H8O3	000547-64-8	9



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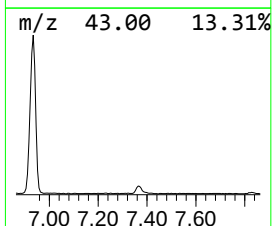
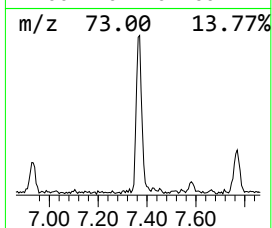
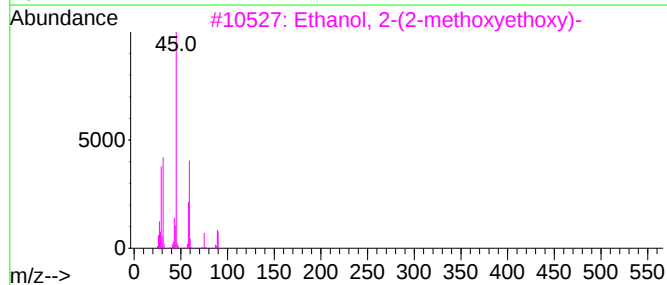
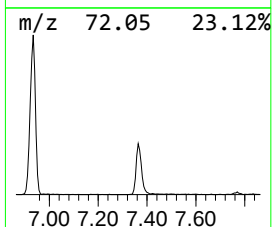
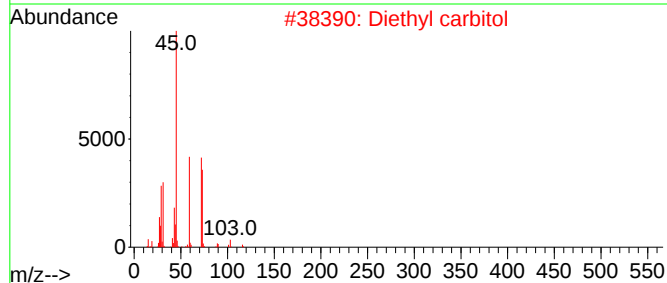
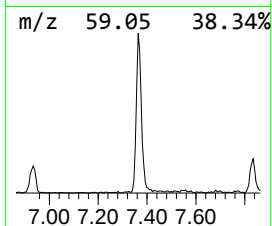
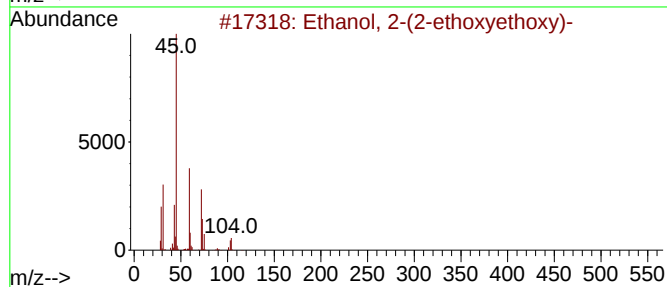
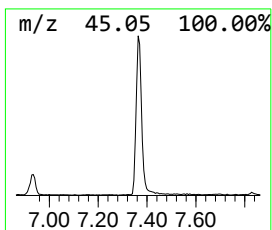
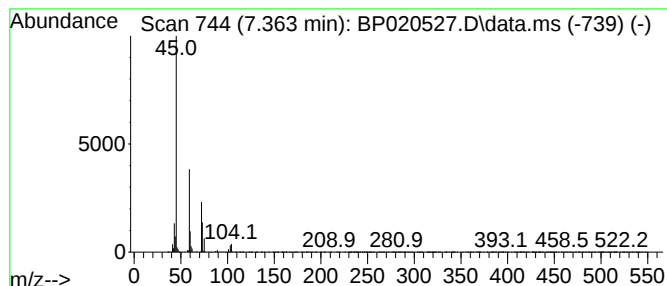
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.363	2.95 ng	212960	1,4-Dichlorobenzene-d4	7.769

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	72
3			Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	45
4			2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	45
5			2-Butanol, 3-methyl-	88	C5H12O	000598-75-4	38



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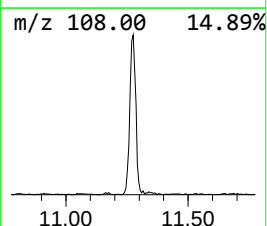
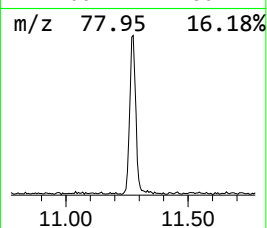
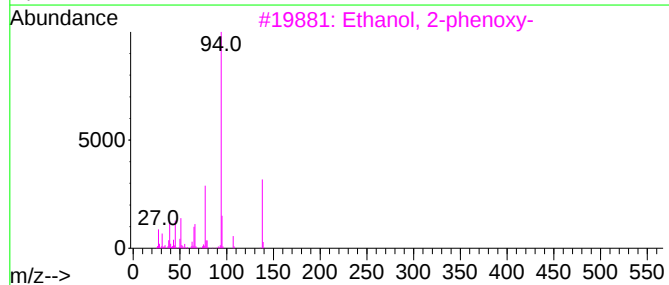
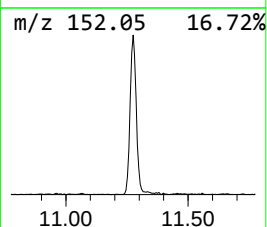
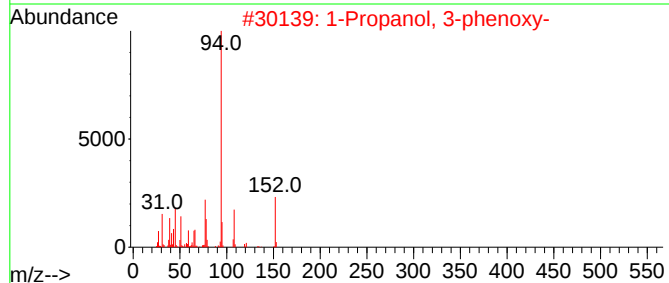
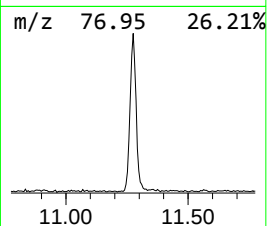
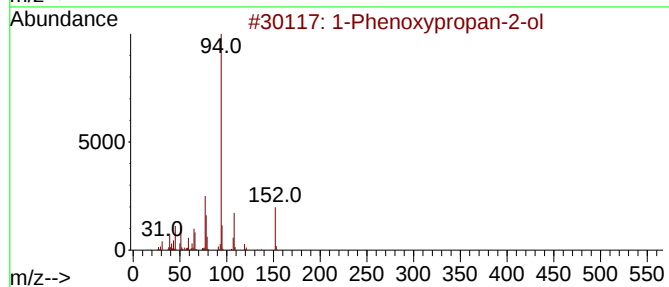
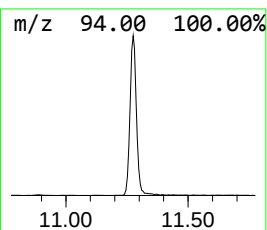
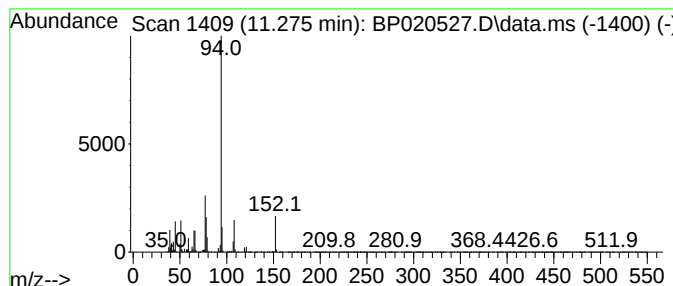
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TIC Integration Parameters: LSCINT.P

Peak Number 4 1-Phenoxypropan-2-ol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.275	5.14 ng	509469	Naphthalene-d8	10.534

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	91
3			Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
4			Carbonic acid, neopentyl phenyl ...	208	C12H16O3	013183-19-2	59
5			1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	59



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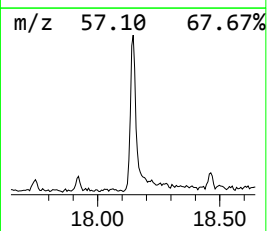
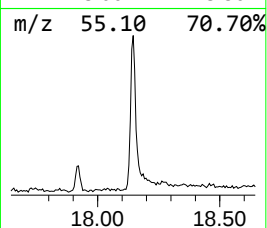
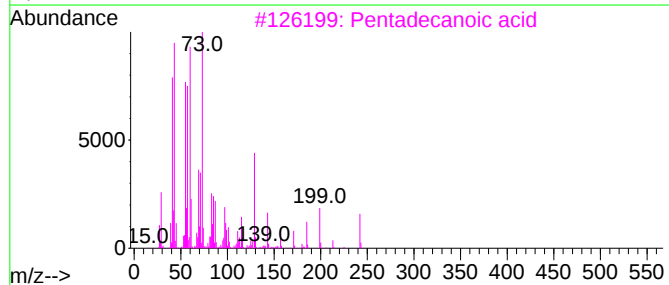
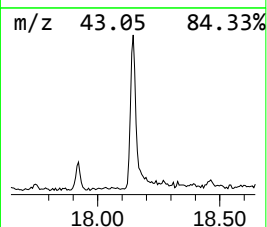
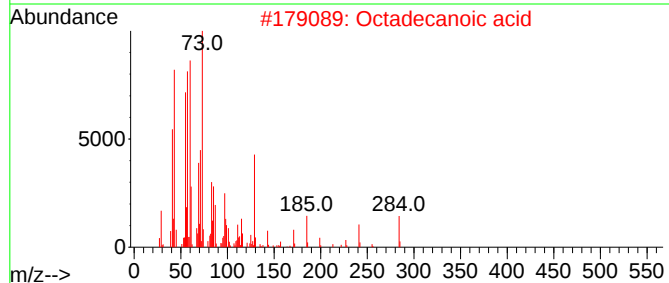
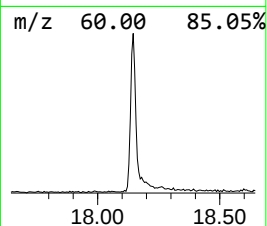
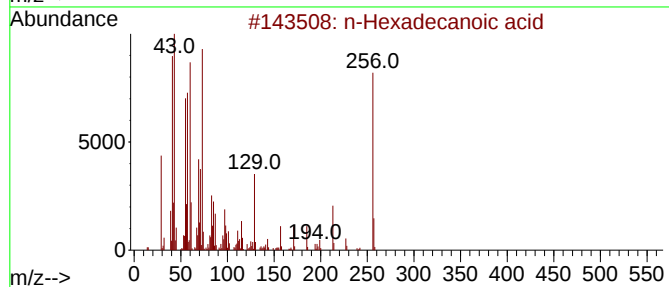
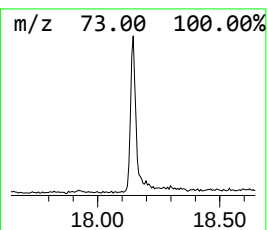
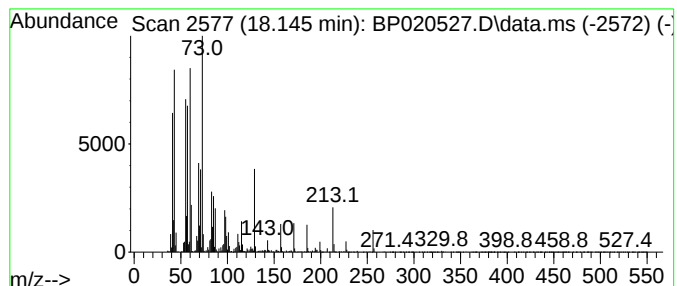
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.145	3.56 ng	539879	Phenanthrene-d10	17.198

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Octadecanoic acid	284	C18H36O2	000057-11-4	90
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4			Tridecanoic acid	214	C13H26O2	000638-53-9	81
5			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	70



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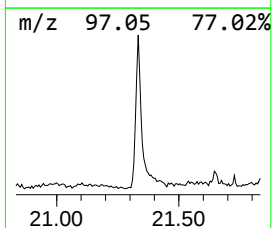
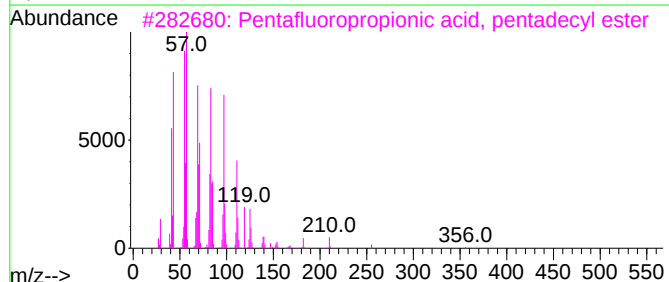
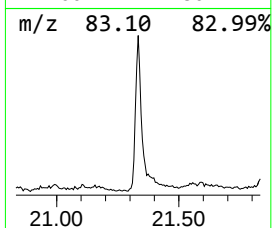
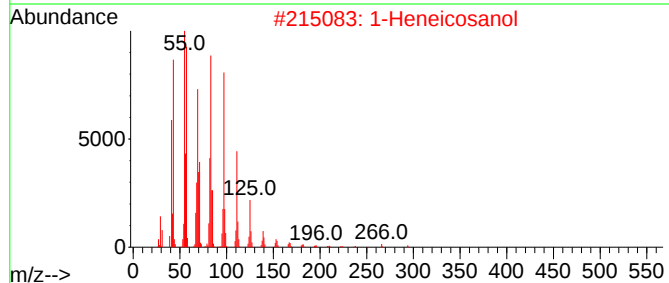
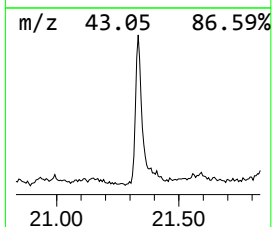
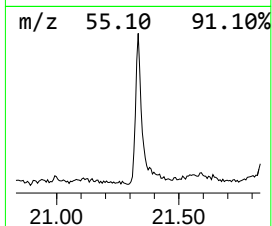
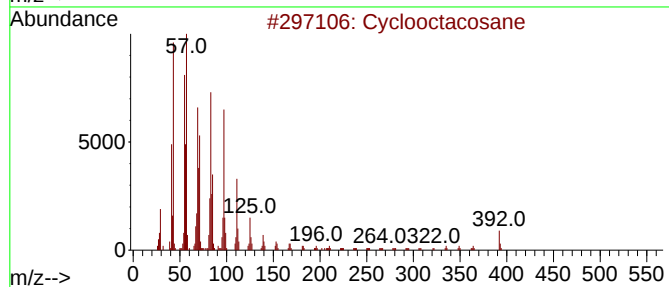
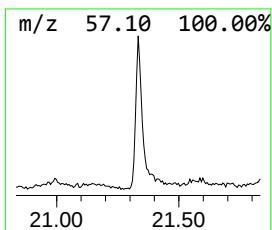
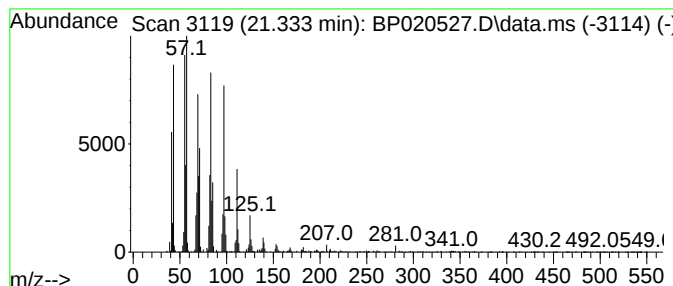
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP052924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Cyclooctacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.333	4.43 ng	750973	Chrysene-d12	21.645

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclooctacosane	392	C28H56	000297-24-5	95
2			1-Heneicosanol	312	C21H44O	015594-90-8	95
3			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
4			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
5			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP060524\
Data File : BP020527.D
Acq On : 05 Jun 2024 22:00
Operator : MA/JU
Sample : P2662-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
WCS-TPR

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...	3.040	50.4	ng	3643070	1	7.769	1444520	20.0
(S)-(+)-1,2-Pro...	3.558	9.1	ng	654489	1	7.769	1444520	20.0
Ethanol, 2-(2-e...	7.363	3.0	ng	212960	1	7.769	1444520	20.0
1-Phenoxypropan...	11.275	5.1	ng	509469	2	10.534	1981710	20.0
n-Hexadecanoic ...	18.145	3.6	ng	539879	4	17.198	3035740	20.0
Cyclooctacosane	21.333	4.4	ng	750973	5	21.645	3387590	20.0