

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021822\
 Data File : BP009214.D
 Acq On : 18 Feb 2022 15:20
 Operator : CG/JU
 Sample : N1573-06
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 MW-1R

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-BP020722.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP009214.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.252	210	215	233	rVB	256781	431920	2.38%	0.657%
2	5.364	398	404	432	rBV	1438328	2785698	15.38%	4.240%
3	6.969	670	677	696	rBV	795510	1785819	9.86%	2.718%
4	7.316	731	736	741	rBV	151136	243584	1.34%	0.371%
5	7.375	741	746	755	rVB	146409	266252	1.47%	0.405%
6	7.563	771	778	792	rBV	211672	440785	2.43%	0.671%
7	7.763	805	812	820	rBV	625171	1062262	5.86%	1.617%
8	8.128	868	874	885	rVB	382974	644844	3.56%	0.982%
9	8.928	1003	1010	1037	rBV	1980080	3921943	21.65%	5.970%
10	10.563	1280	1288	1294	rBV	754459	1429414	7.89%	2.176%
11	12.763	1654	1662	1673	rBV	236620	413963	2.28%	0.630%
12	13.028	1699	1707	1722	rBV	6584150	10758971	59.38%	16.377%
13	13.263	1740	1747	1763	rVB	1011885	1667922	9.21%	2.539%
14	14.410	1935	1942	1952	rBV	1426437	2185621	12.06%	3.327%
15	15.240	2076	2083	2095	rVB	253582	377980	2.09%	0.575%
16	15.781	2170	2175	2185	rBV	226293	342015	1.89%	0.521%
17	15.916	2191	2198	2215	rBV	5244717	8658195	47.79%	13.179%
18	17.175	2406	2412	2426	rVB	1725892	2729434	15.07%	4.155%
19	17.839	2520	2525	2531	rBV	253367	316921	1.75%	0.482%
20	19.739	2842	2848	2859	rBV	13985431	18117419	100.00%	27.578%
21	21.275	3104	3109	3120	rBV	2317938	3611026	19.93%	5.497%
22	23.663	3509	3515	3528	rVB2	1575704	3504091	19.34%	5.334%

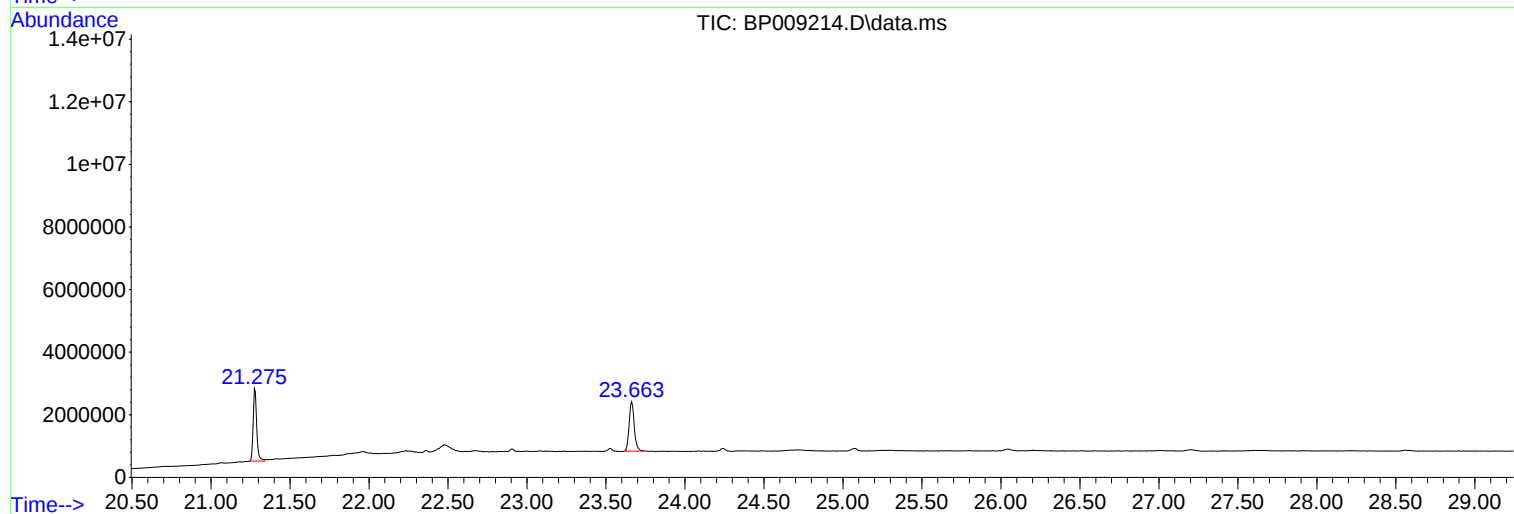
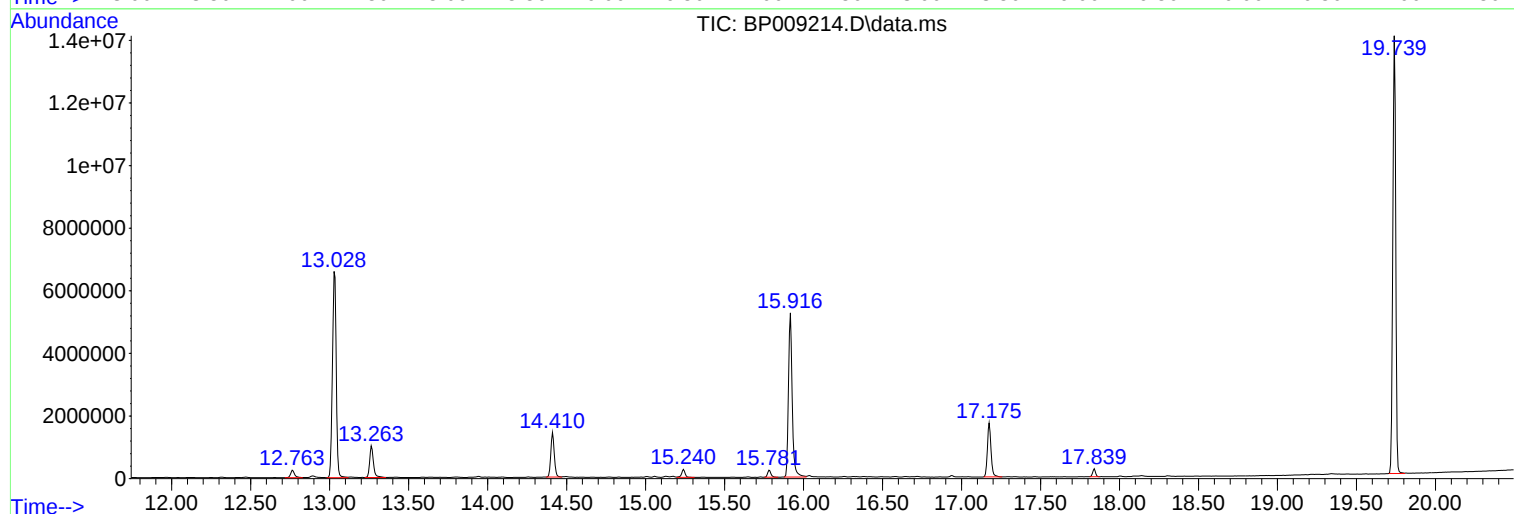
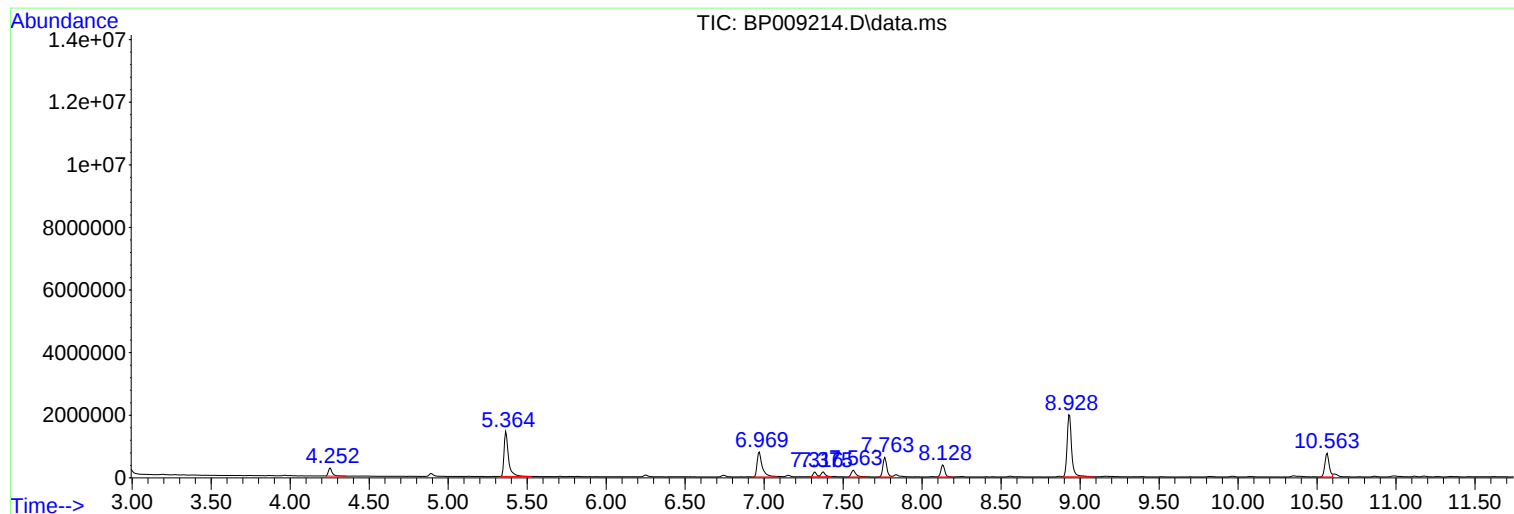
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BNA_P
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP020722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Data File : BP009214.D
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Operator : CG/JU
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Instrument :
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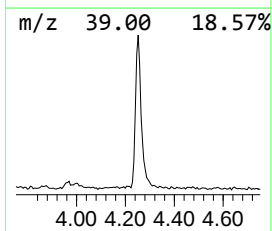
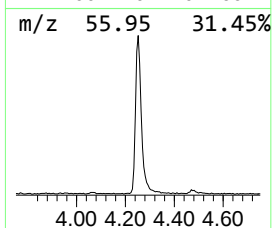
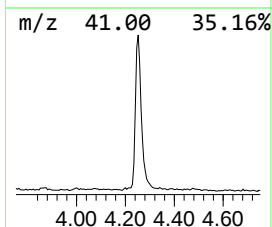
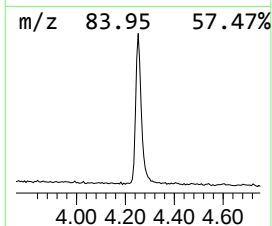
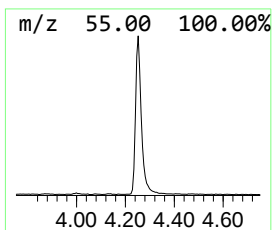
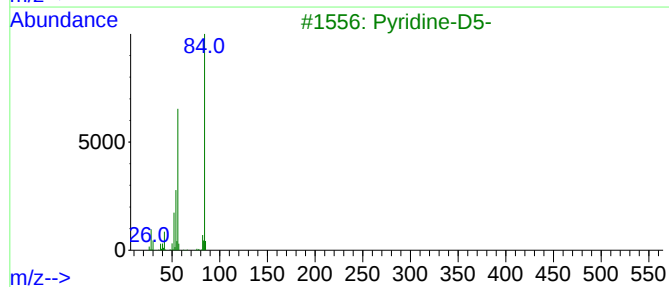
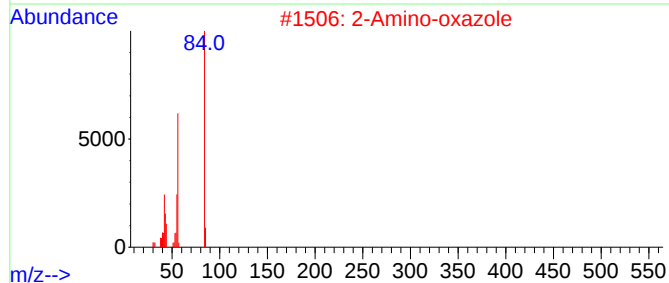
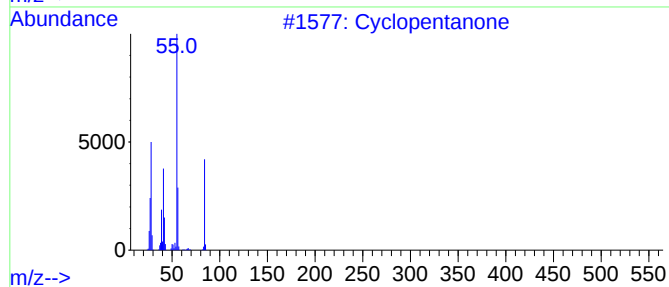
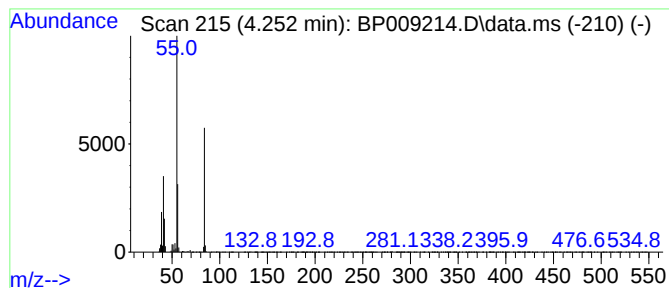
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Cyclopentanone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.252	8.13 ng	431920	1,4-Dichlorobenzene-d4	7.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentanone	84	C5H8O	000120-92-3	91
2			2-Amino-oxazole	84	C3H4N2O	004570-45-0	53
3			Pyridine-D5-	84	C5D5N	007291-22-7	52
4			2(5H)-Furanone	84	C4H4O2	000497-23-4	52
5			2H-Pyran, 3,4-dihydro-	84	C5H8O	000110-87-2	42



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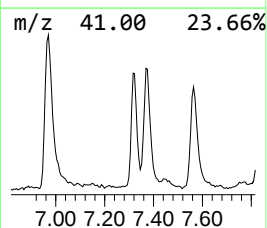
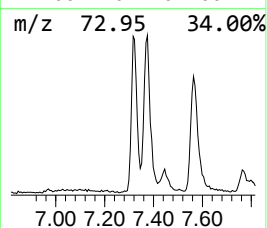
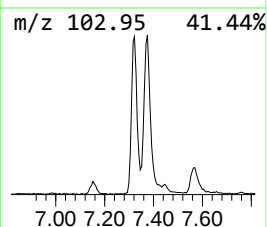
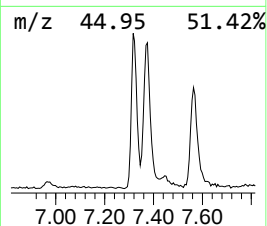
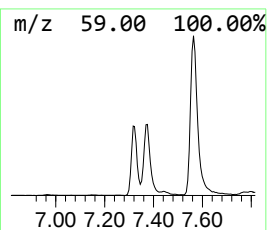
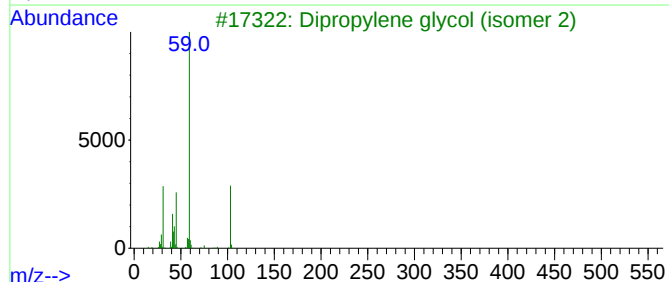
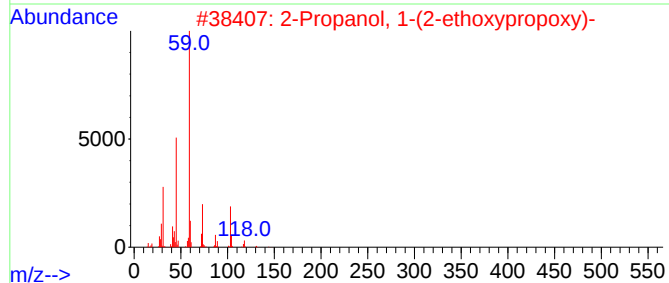
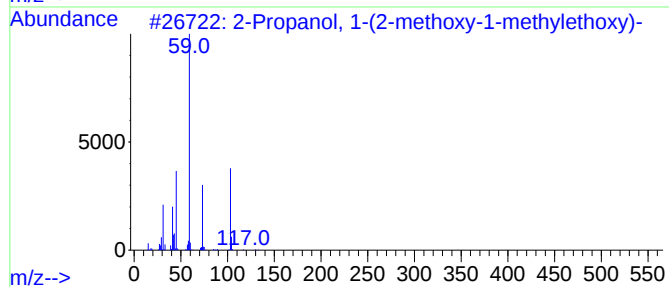
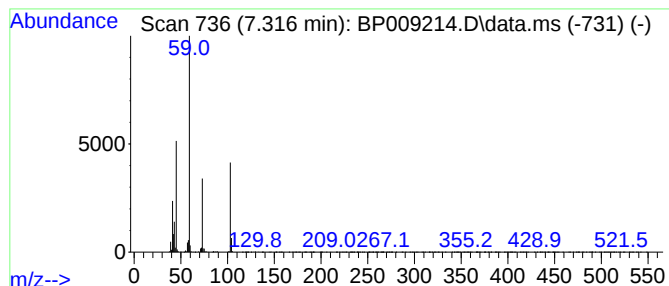
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Propanol, 1-(2-methoxy-1-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.316	4.59 ng	243584	1,4-Dichlorobenzene-d4	7.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	72		
2	2-Propanol, 1-(2-ethoxypropoxy)-	162	C8H18O3	010143-32-5	64		
3	Dipropylene glycol (isomer 2)	134	C6H14O3	1000506-25-4	53		
4	Dipropylene glycol (isomer 3)	134	C6H14O3	1000506-25-5	53		
5	1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	53		



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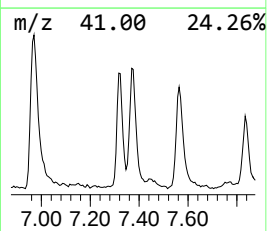
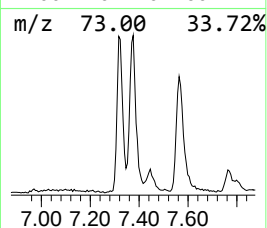
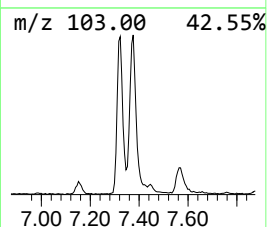
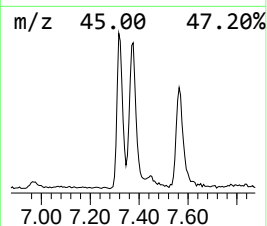
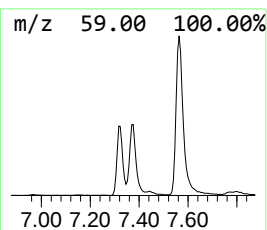
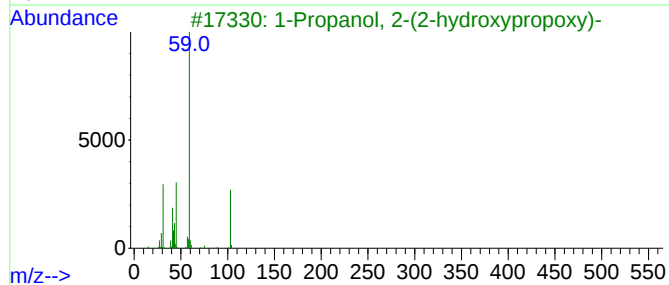
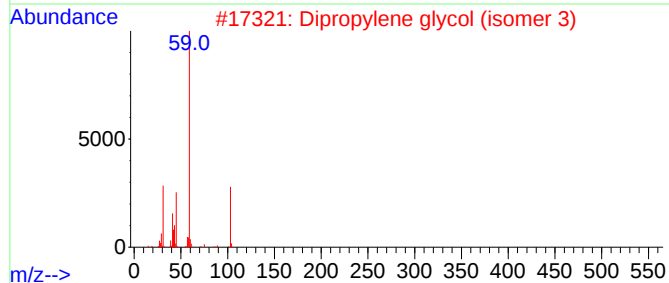
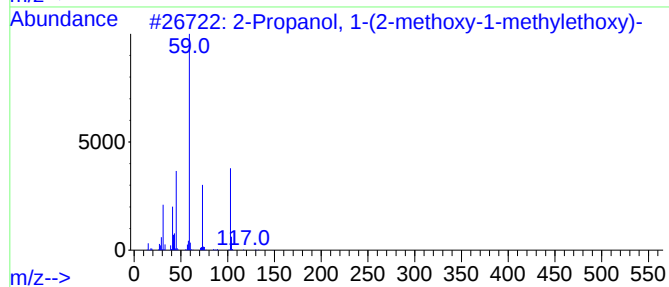
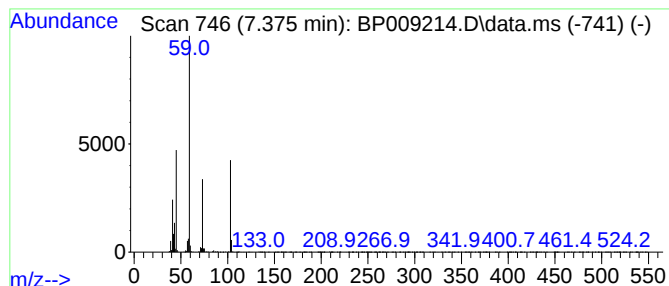
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Dipropylene glycol (isomer 3) Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.375	5.01 ng	266252	1,4-Dichlorobenzene-d4	7.763

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	90
2		Dipropylene glycol (isomer 3)	134	C6H14O3	1000506-25-5	53
3		1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	53
4		Dipropylene glycol (isomer 2)	134	C6H14O3	1000506-25-4	53
5		1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	53



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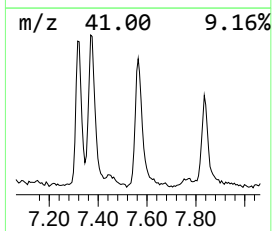
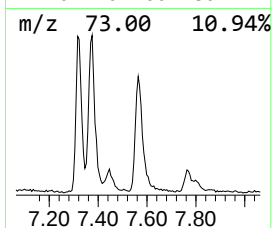
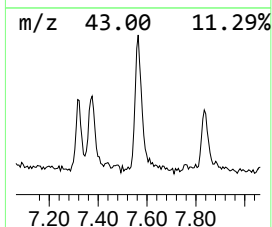
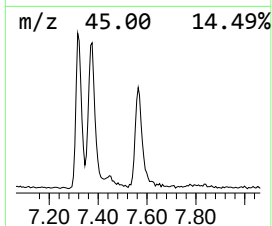
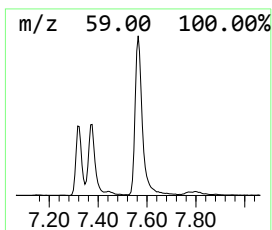
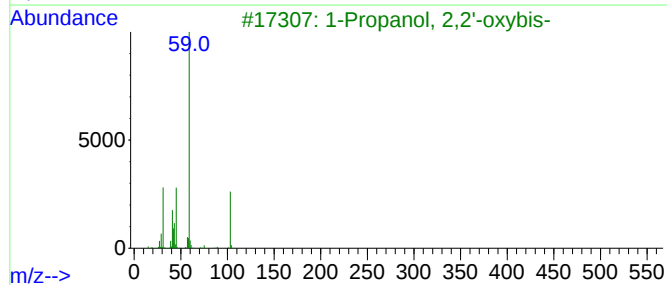
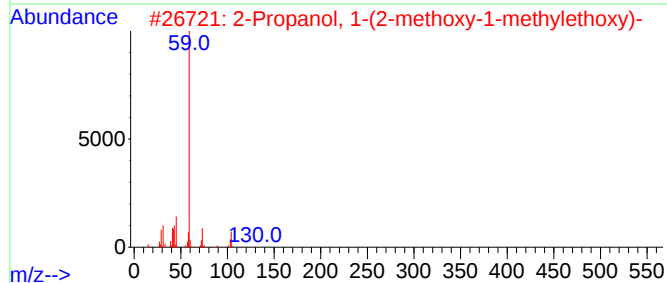
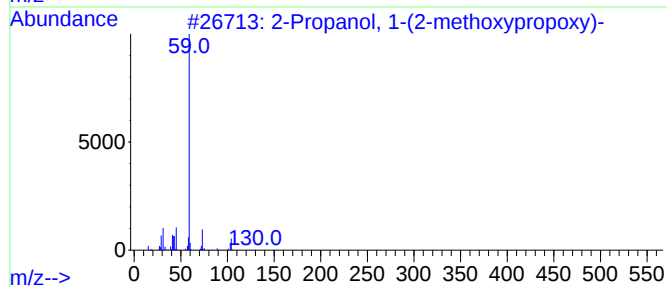
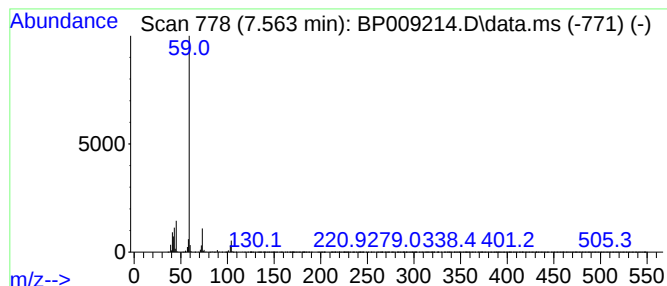
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Peak Number 4 2-Propanol, 1-(2-methoxypro... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.563	8.30 ng	440785	1,4-Dichlorobenzene-d4	7.763

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Propanol, 1-(2-methoxypropoxy)-	148	C7H16O3	013429-07-7	83
2		2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	83
3		1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	64
4		1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	50
5		2-Propanol, 1-[1-methyl-2-(2-pro...	174	C9H18O3	055956-25-7	43



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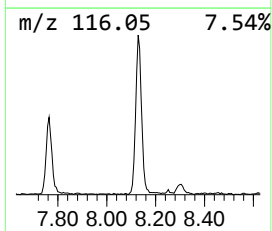
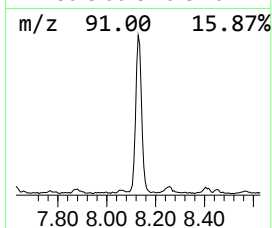
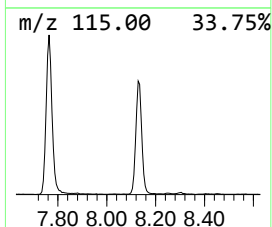
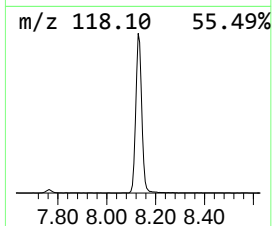
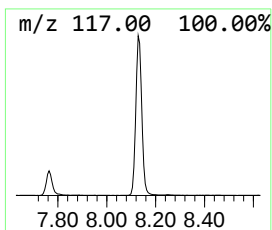
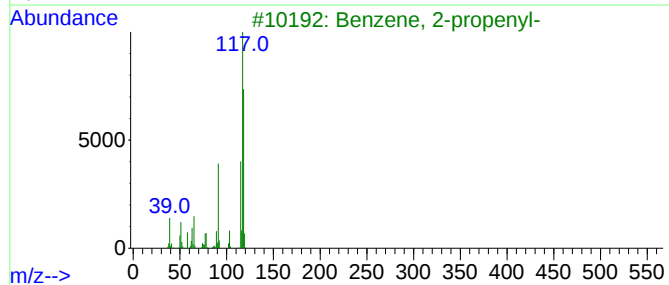
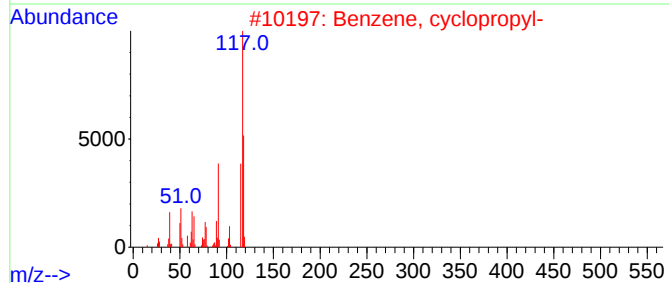
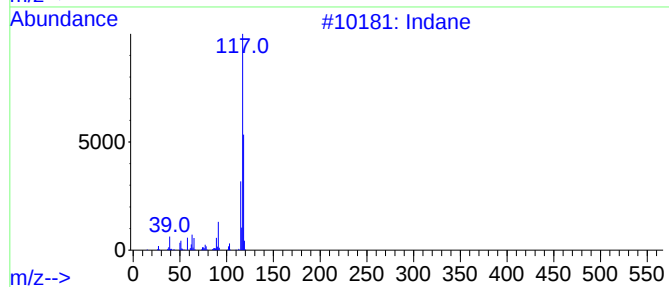
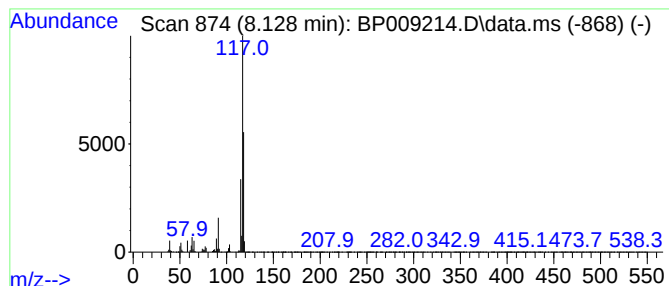
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Indane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.128	12.14 ng	644844	1,4-Dichlorobenzene-d4	7.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	93
2			Benzene, cyclopropyl-	118	C9H10	000873-49-4	72
3			Benzene, 2-propenyl-	118	C9H10	000300-57-2	64
4			Benzene, 1,1'-(1,5-hexadiene-1,6...	234	C18H18	004439-45-6	59
5			7-Methylenecycloocta-1,3,5-triene	118	C9H10	002570-13-0	59



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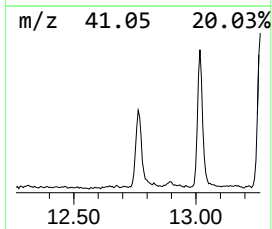
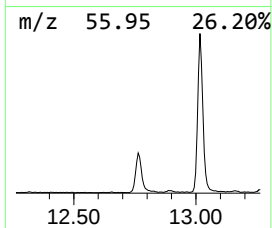
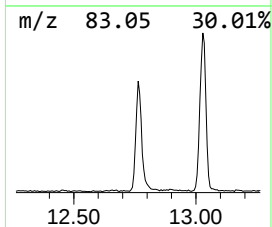
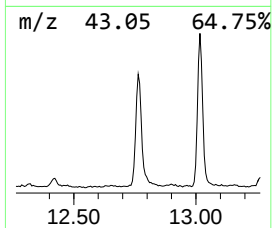
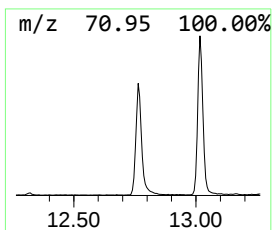
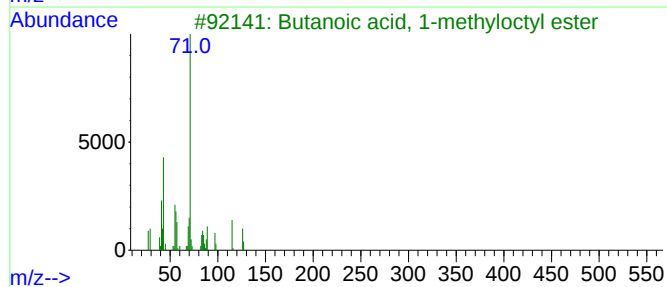
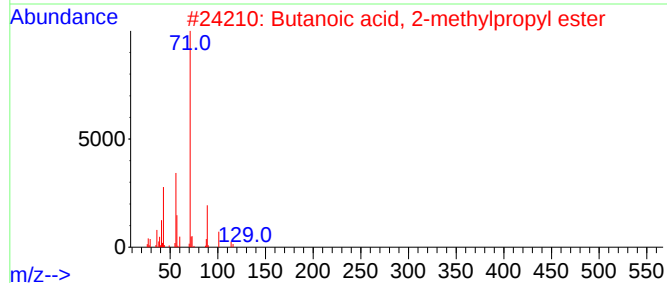
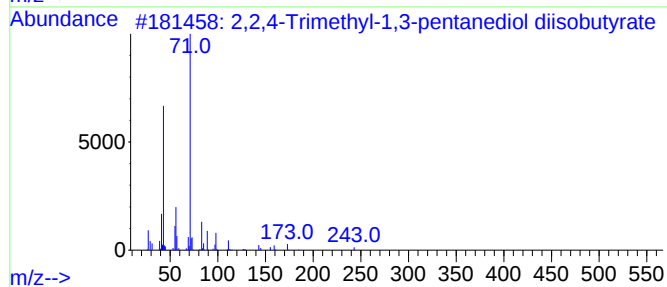
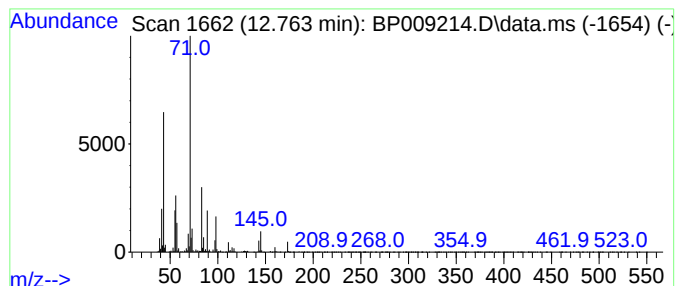
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 2,2,4-Trimethyl-1,3-pentane... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.763	3.79 ng	413963	Acenaphthene-d10	14.410

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,2,4-Trimethyl-1,3-pentanediol ...	286	C16H30O4	006846-50-0	64
2			Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	42
3			Butanoic acid, 1-methyloctyl ester	214	C13H26O2	069727-42-0	37
4			Butane, 2-iodo-3-methyl-	198	C5H11I	018295-27-7	35
5			Butanoic acid, 3-butenyl ester	142	C8H14O2	021698-32-8	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021822\
Data File : BP009214.D
Acq On : 18 Feb 2022 15:20
Operator : CG/JU
Sample : N1573-06
Misc :
ALS Vial : 7 Sample Multiplier: 1

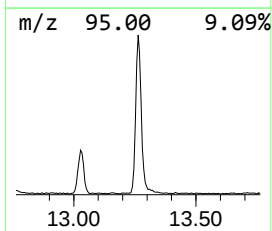
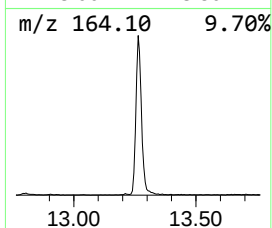
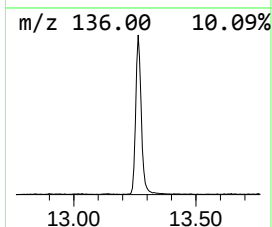
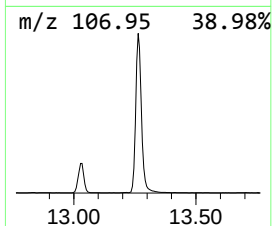
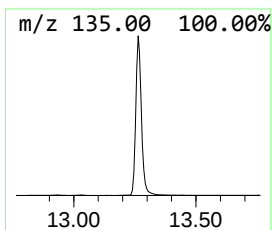
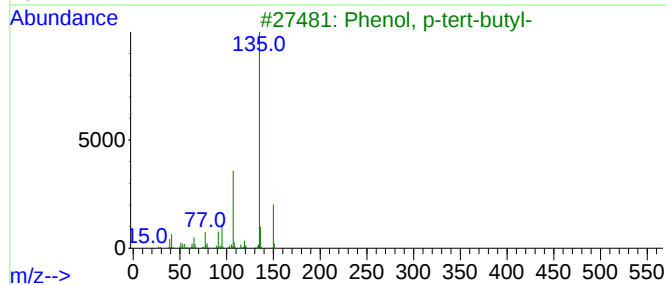
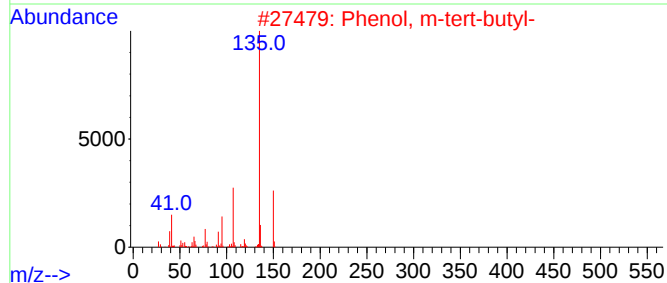
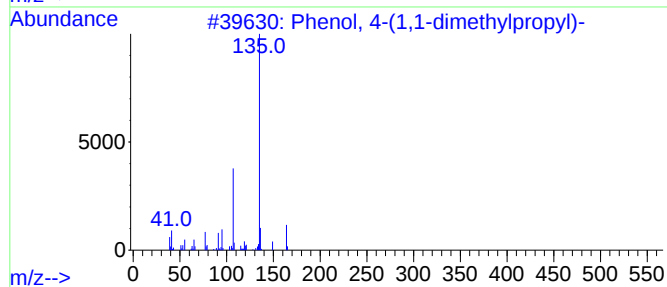
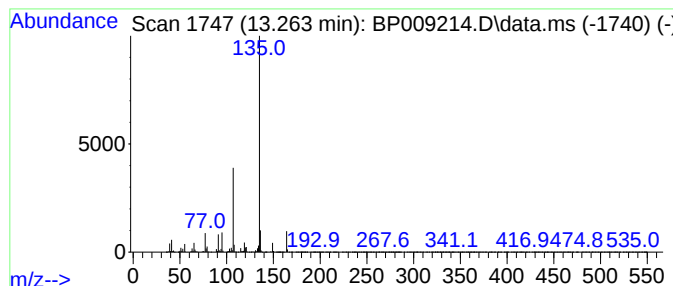
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP020722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Phenol, 4-(1,1-dimethylprop... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD			R.T.
13.263	15.26 ng	1667920	Acenaphthene-d10			14.410
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Phenol, 4-(1,1-dimethylpropyl)-		164	C11H16O	000080-46-6	97
2	Phenol, m-tert-butyl-		150	C10H14O	000585-34-2	86
3	Phenol, p-tert-butyl-		150	C10H14O	000098-54-4	80
4	Hexestrol, O-trifluoroacetyl-		366	C20H21F3O3	1000365-31-7	64
5	Hexestrol, O-isopropoxyloxycarbonyl-		356	C22H28O4	1000487-68-4	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021822\
Data File : BP009214.D
Acq On : 18 Feb 2022 15:20
Operator : CG/JU
Sample : N1573-06
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-1R

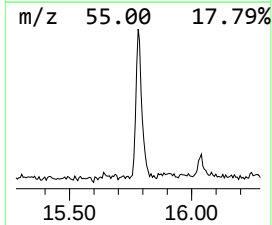
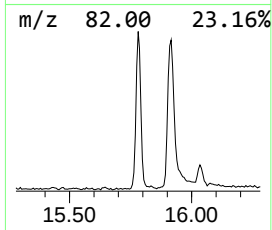
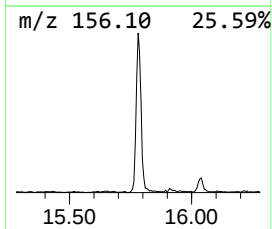
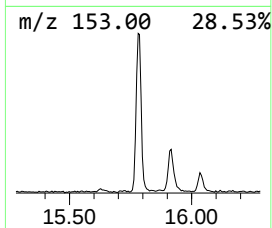
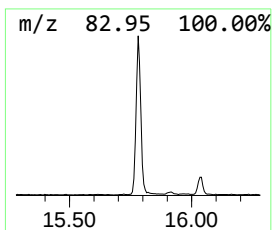
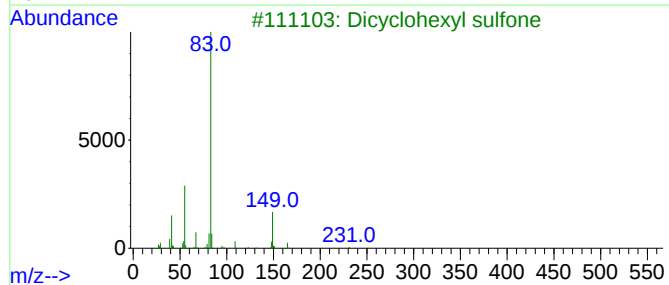
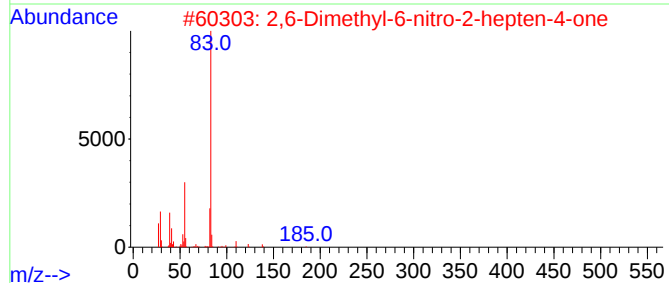
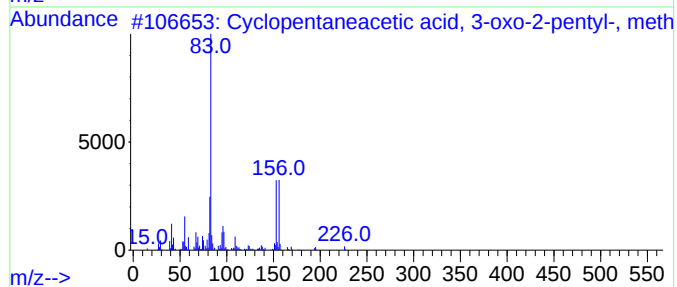
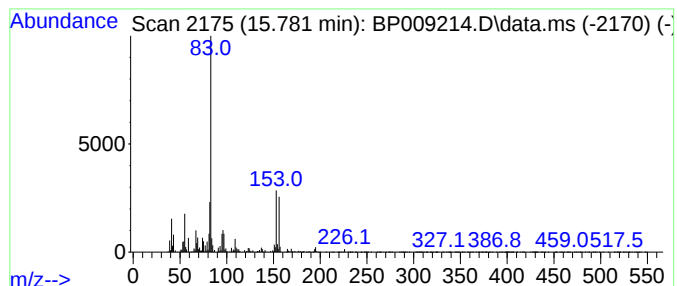
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Cyclopentaneacetic acid, 3-... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.781	3.13 ng	342015	Acenaphthene-d10	14.410

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentaneacetic acid, 3-oxo-2...	226	C13H22O3	024851-98-7	98
2			2,6-Dimethyl-6-nitro-2-hepten-4-one	185	C9H15NO3	073583-56-9	43
3			Dicyclohexyl sulfone	230	C12H22O2S	1000451-31-4	38
4			6-Hydroxy-10a-methyl-4,7-dimethy...	376	C20H24O7	1798297-60-5	38
5			Hexanal di-cis-3-hexenyl acetal	282	C18H34O2	1000430-94-7	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021822\
Data File : BP009214.D
Acq On : 18 Feb 2022 15:20
Operator : CG/JU
Sample : N1573-06
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-1R

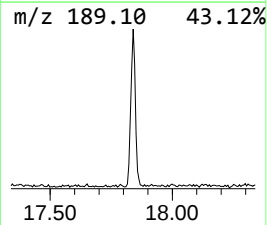
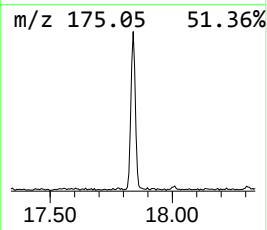
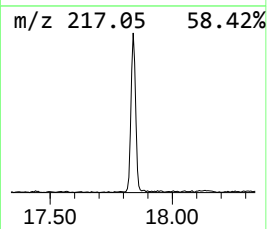
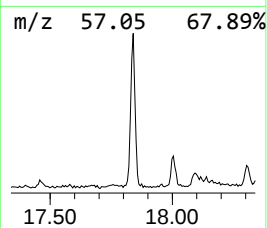
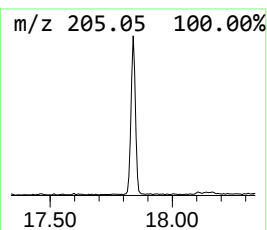
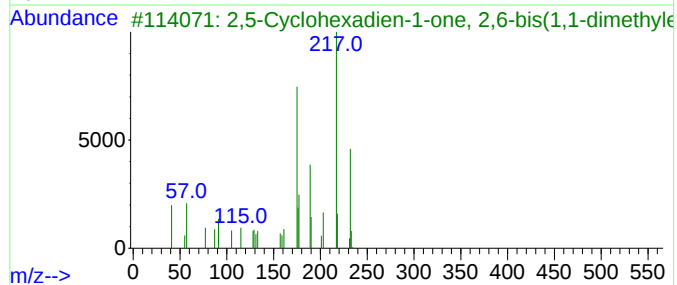
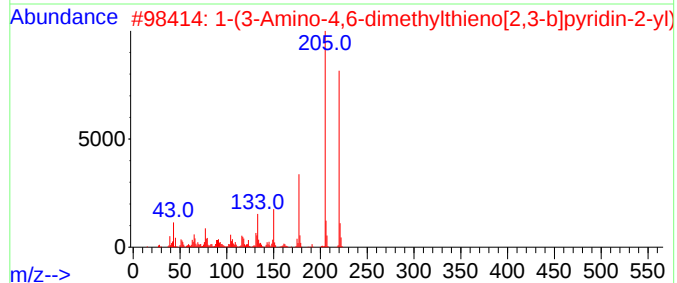
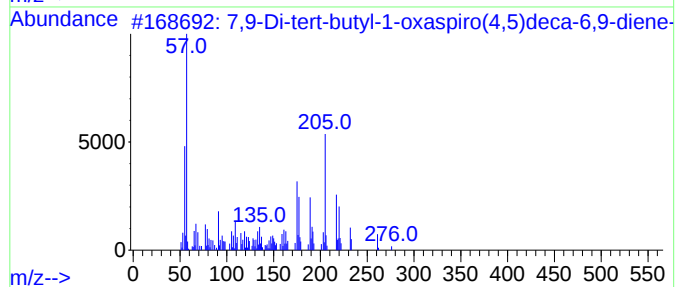
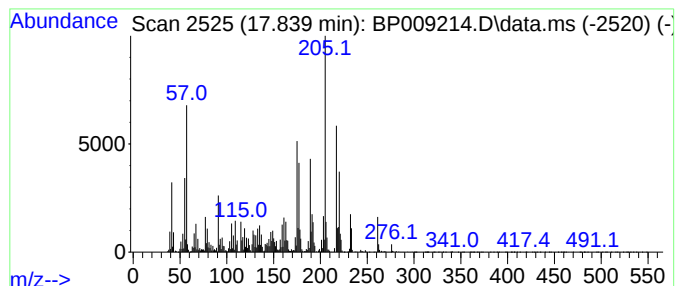
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP020722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 7,9-Di-tert-butyl-1-oxaspiro... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.839	2.32 ng	316921	Phenanthrene-d10	17.175

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	99		
2	1-(3-Amino-4,6-dimethylthieno[2,...	220	C11H12N2OS	052505-42-7	50		
3	2,5-Cyclohexadien-1-one, 2,6-bis...	232	C16H24O	006738-27-8	49		
4	Ethanone, 1-(5,6,7,8-tetrahydro-...	220	C14H20O2	071596-88-8	45		
5	2,5-di-tert-Butyl-1,4-benzoquinone	220	C14H20O2	002460-77-7	45		



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021822\
 Data File : BP009214.D
 Acq On : 18 Feb 2022 15:20
 Operator : CG/JU
 Sample : N1573-06
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 MW-1R

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP020722.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
Cyclopentanone	4.252	8.1	ng	431920	1	7.763	1062260	20.0
2-Propanol, 1-(...	7.316	4.6	ng	243584	1	7.763	1062260	20.0
Dipropylene gly...	7.375	5.0	ng	266252	1	7.763	1062260	20.0
2-Propanol, 1-(...	7.563	8.3	ng	440785	1	7.763	1062260	20.0
Indane	8.128	12.1	ng	644844	1	7.763	1062260	20.0
2,2,4-Trimethyl...	12.763	3.8	ng	413963	3	14.410	2185620	20.0
Phenol, 4-(1,1-...	13.263	15.3	ng	1667920	3	14.410	2185620	20.0
Cyclopentaneace...	15.781	3.1	ng	342015	3	14.410	2185620	20.0
7,9-Di-tert-but...	17.839	2.3	ng	316921	4	17.175	2729430	20.0