

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP052821\
 Data File : BP005641.D
 Acq On : 28 May 2021 16:22
 Operator : CG/JU
 Sample : M2560-01
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 S1-COMP-A-B-C-D

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-BP052721.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP005641.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.116	3	5	10	rVB	1899635	1921660	15.20%	2.843%
2	3.158	10	12	22	rVB	121641	167835	1.33%	0.248%
3	5.081	332	339	347	rBV2	130242	203788	1.61%	0.302%
4	5.546	411	418	428	rBV	3926229	5618468	44.43%	8.313%
5	7.146	682	690	702	rBV	3752345	5989343	47.36%	8.862%
6	7.987	826	833	840	rBV	851778	1313258	10.38%	1.943%
7	9.146	1021	1030	1040	rBV	2205151	3721655	29.43%	5.507%
8	10.792	1302	1310	1322	rBV	1065196	1799110	14.23%	2.662%
9	13.239	1719	1726	1734	rBV	5536681	8079929	63.89%	11.956%
10	13.404	1750	1754	1764	rBV4	73936	137592	1.09%	0.204%
11	14.063	1857	1866	1870	rBV2	589392	1199087	9.48%	1.774%
12	14.357	1911	1916	1921	rBV4	146665	279509	2.21%	0.414%
13	14.445	1927	1931	1937	rVB	409623	640741	5.07%	0.948%
14	14.516	1939	1943	1948	rBV4	89902	164068	1.30%	0.243%
15	14.604	1949	1958	1967	rBV	1657883	2872756	22.72%	4.251%
16	14.704	1971	1975	1979	rVV4	94556	152161	1.20%	0.225%
17	15.133	2044	2048	2051	rBV2	175042	288844	2.28%	0.427%
18	15.269	2068	2071	2075	rVB5	184063	234113	1.85%	0.346%
19	15.398	2088	2093	2100	rBV2	570373	876084	6.93%	1.296%
20	16.092	2205	2211	2216	rBV	5113784	7273709	57.52%	10.763%
21	17.351	2421	2425	2430	rBV	1888007	2785006	22.02%	4.121%
22	19.898	2853	2858	2863	rVB	10252934	12645874	100.00%	18.712%
23	21.121	3063	3066	3075	rVB	1284702	1553442	12.28%	2.299%
24	21.415	3111	3116	3121	rBV	2733142	3737806	29.56%	5.531%
25	23.857	3525	3531	3540	rVB2	1912970	3927189	31.06%	5.811%

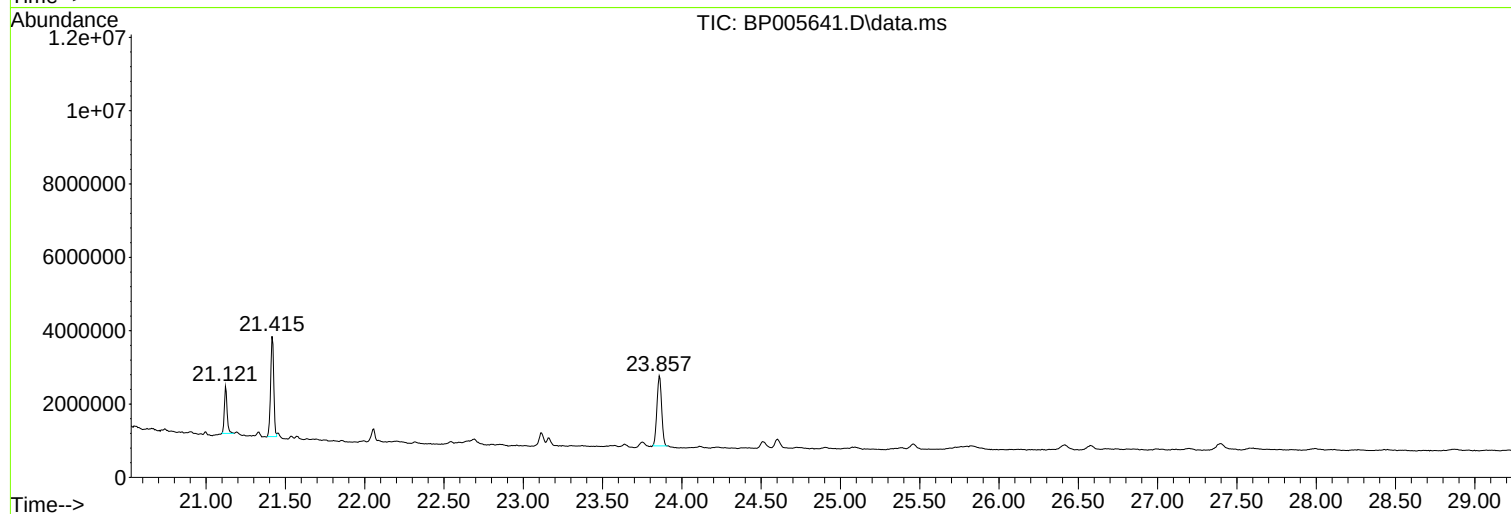
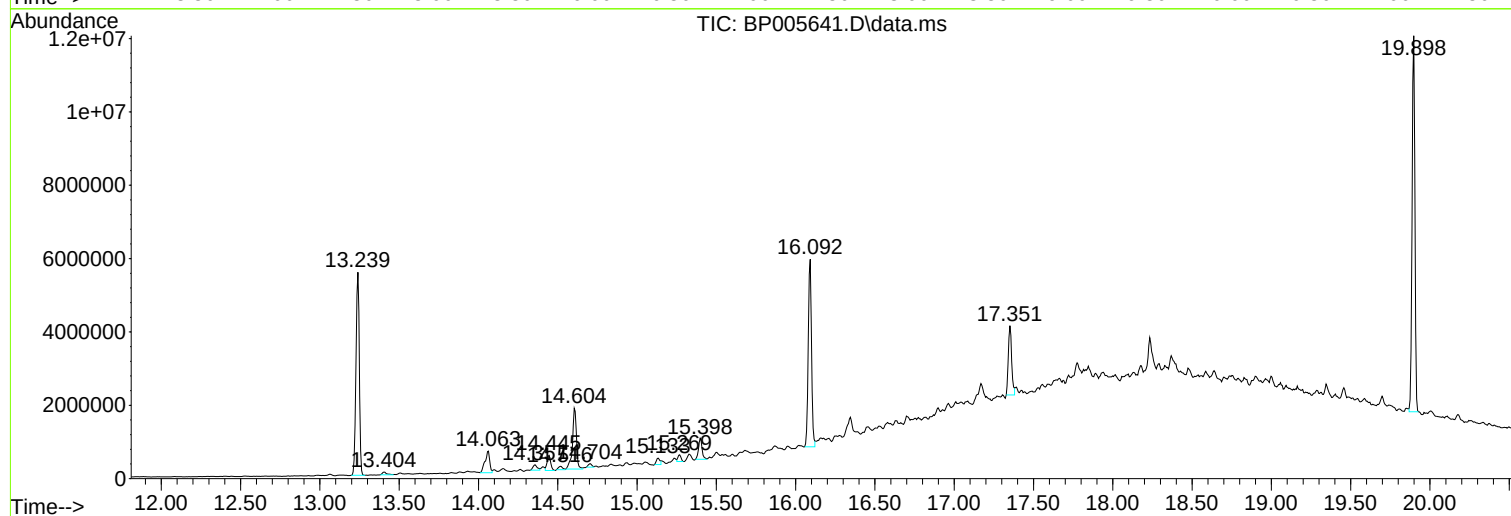
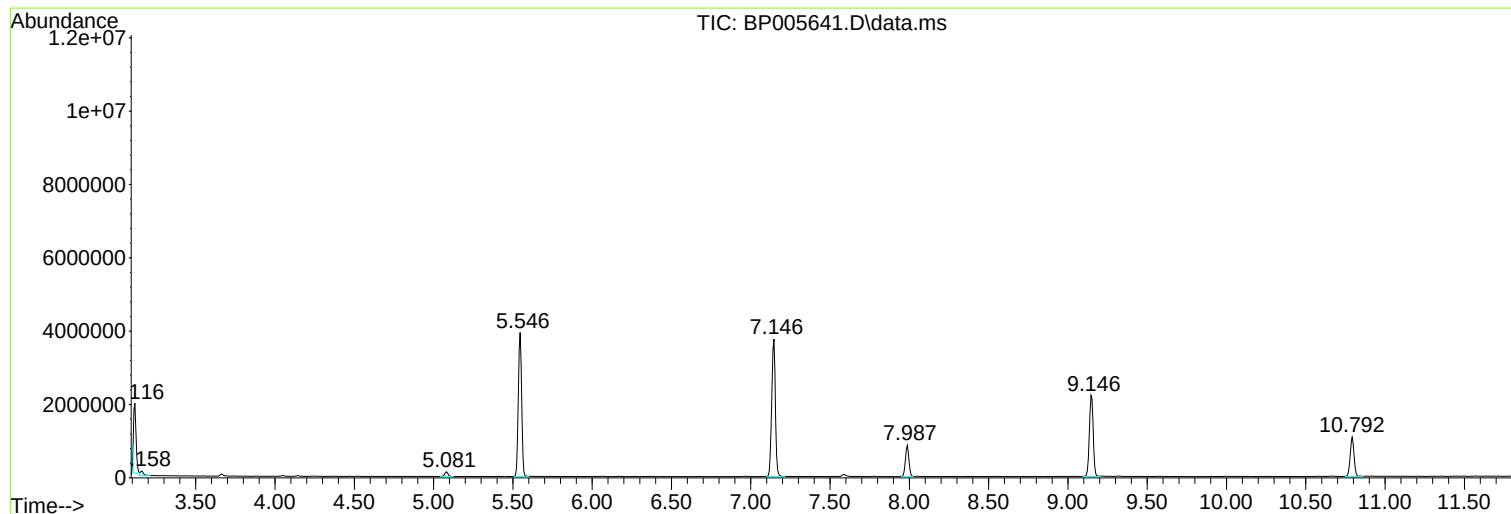
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP052721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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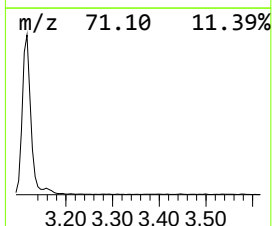
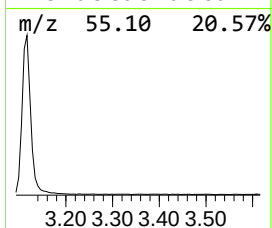
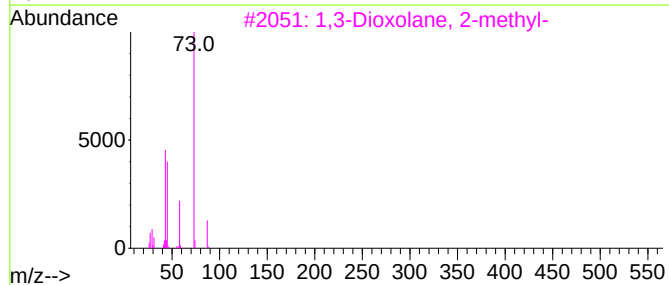
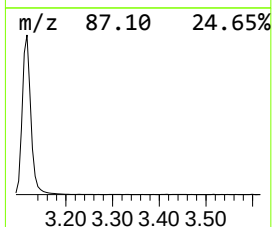
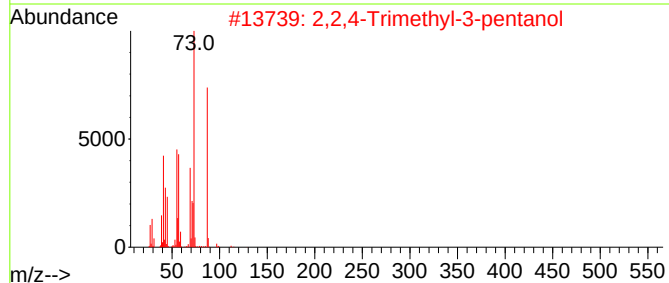
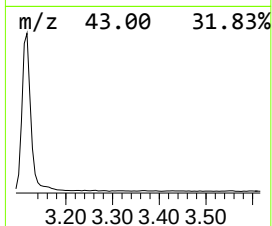
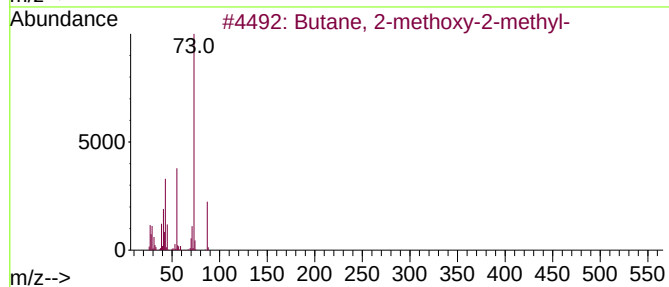
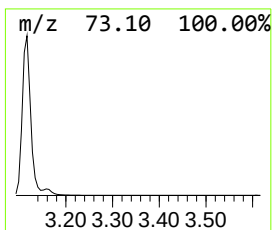
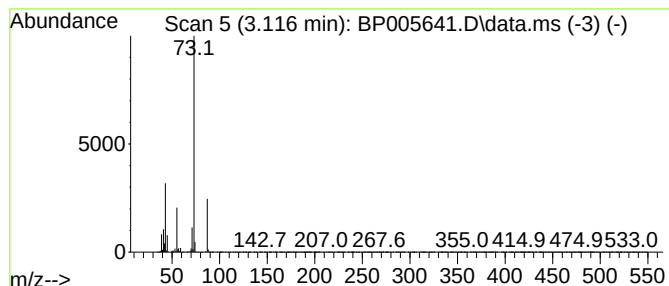
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.116	29.27 ng	1921660	1,4-Dichlorobenzene-d4	7.987

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22



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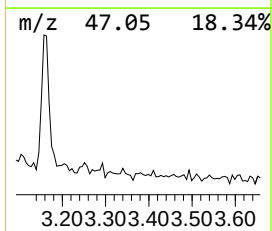
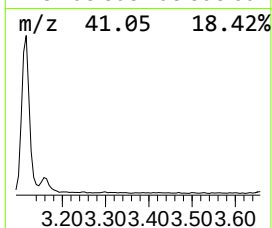
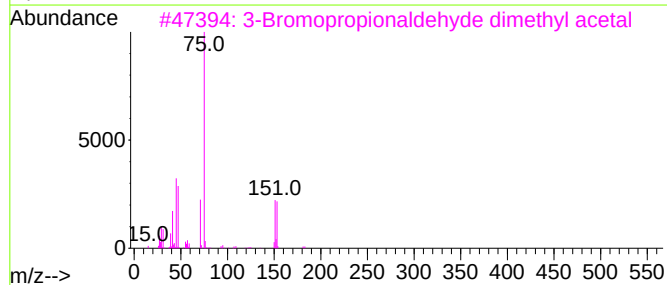
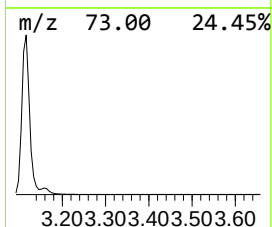
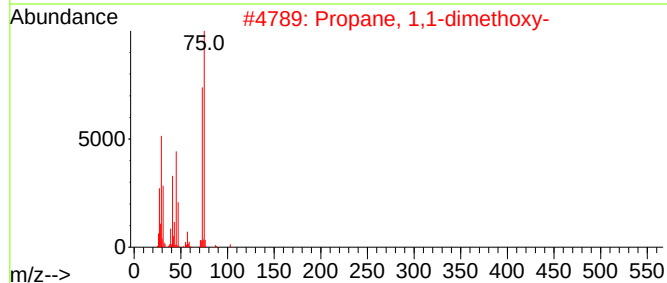
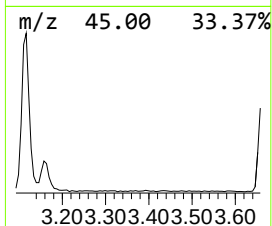
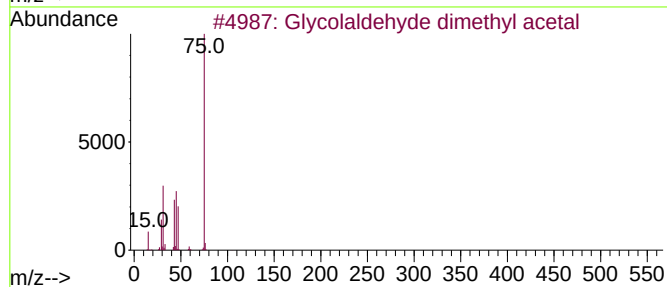
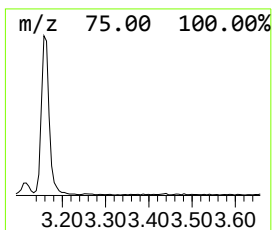
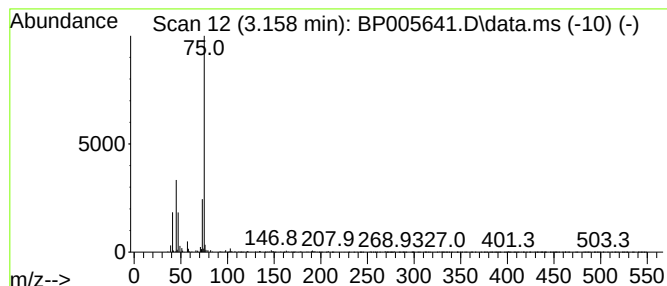
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Peak Number 2 unknown3.15 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.158	2.56 ng	167835	1,4-Dichlorobenzene-d4	7.987

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Glycolaldehyde dimethyl acetal	106	C4H10O3	030934-97-5	45
2			Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	38
3			3-Bromopropionaldehyde dimethyl ...	182	C5H11BrO2	036255-44-4	36
4			2-Propanol, 1,1-dimethoxy-, acetate	162	C7H14O4	074495-37-7	33
5			4-(3-Fluoro-phenyl)-6-methyl-2-o...	324	C15H17FN2O3S	1000276-15-0	9



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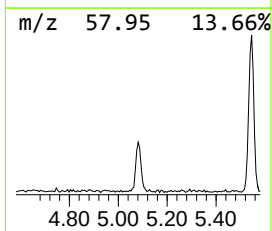
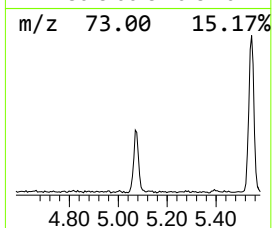
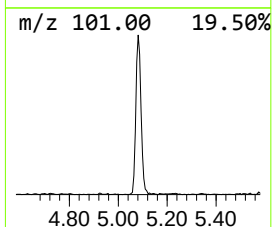
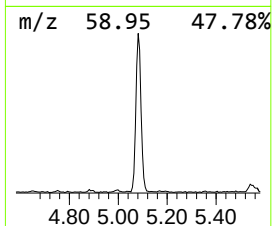
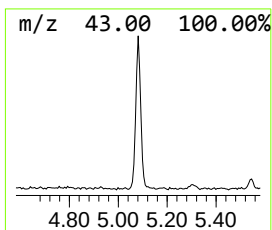
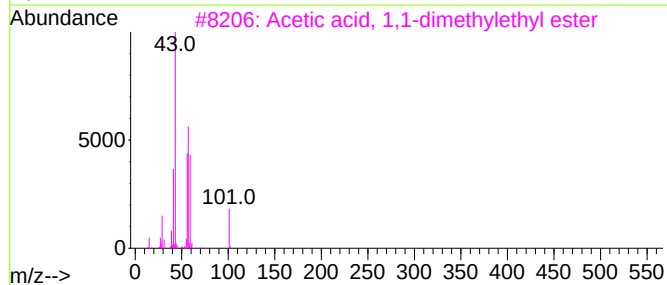
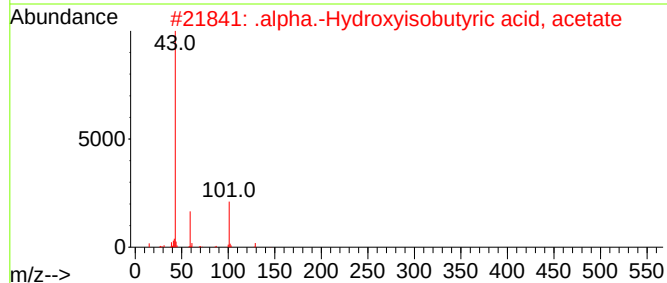
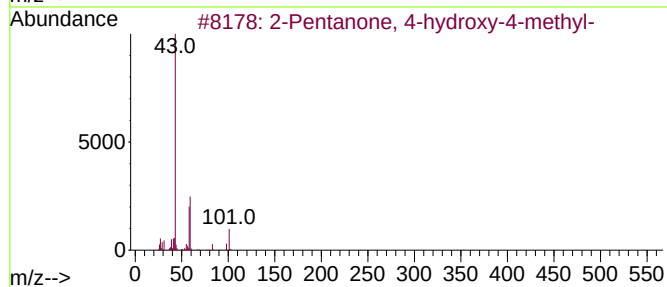
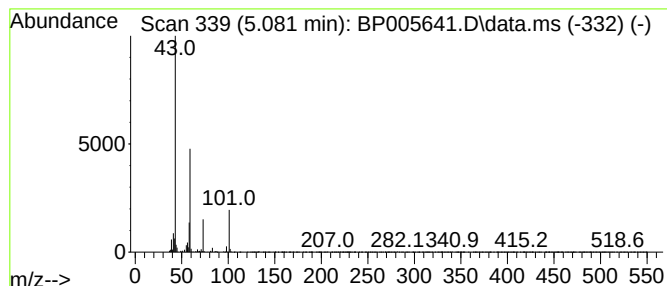
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TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.081	3.10 ng	203788	1,4-Dichlorobenzene-d4	7.987

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			.alpha.-Hydroxyisobutyric acid, ...	146	C6H10O4	1000374-31-3	42
3			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	36
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
5			2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	16



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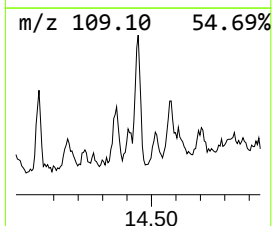
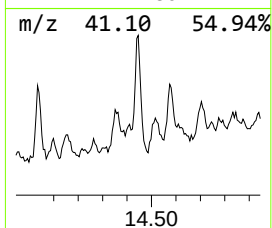
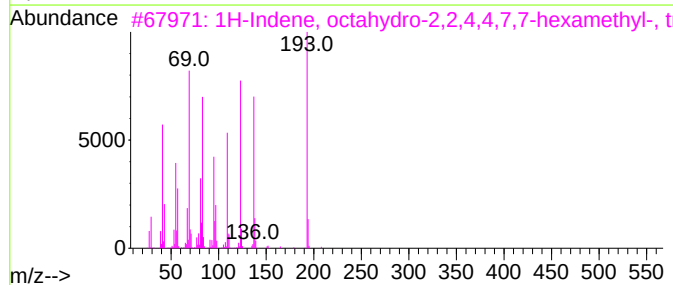
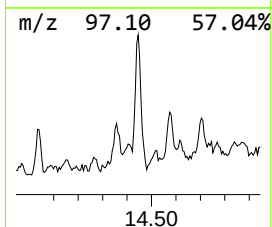
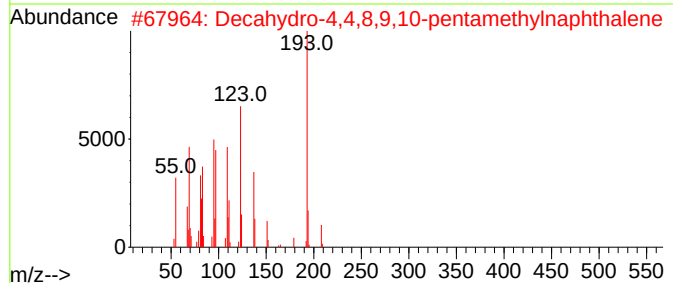
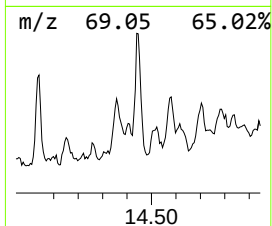
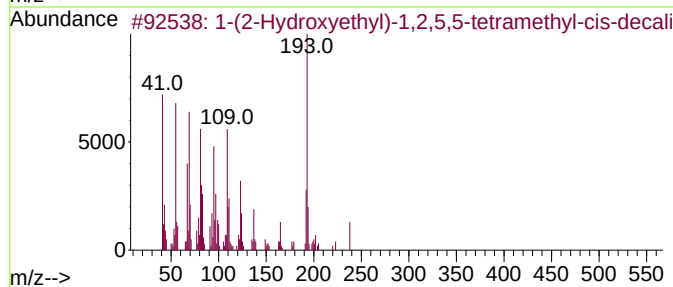
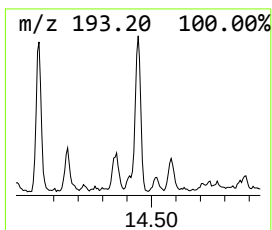
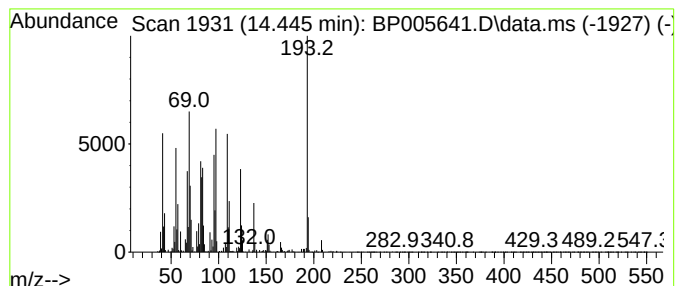
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Peak Number 4 1-(2-Hydroxyethyl)-1,2,5,5-... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.445	4.46 ng	640741	Acenaphthene-d10	14.604

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(2-Hydroxyethyl)-1,2,5,5-tetra...	238	C16H30O	1000298-97-4	56		
2	Decahydro-4,4,8,9,10-pentamethyl...	208	C15H28	080655-44-3	46		
3	1H-Indene, octahydro-2,2,4,4,7,7...	208	C15H28	054832-83-6	37		
4	2-Phenylindolizine	193	C14H11N	025379-20-8	25		
5	Borinic acid, diethyl-, 3,3,5-tr...	208	C13H25BO	057387-76-5	17		



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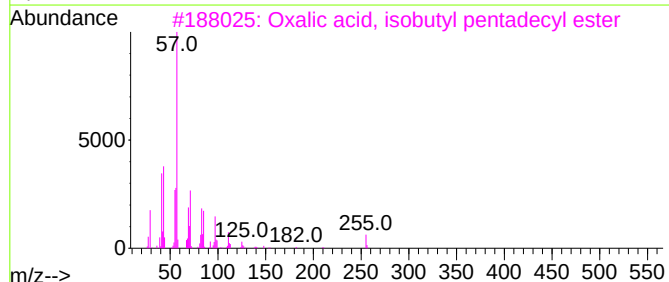
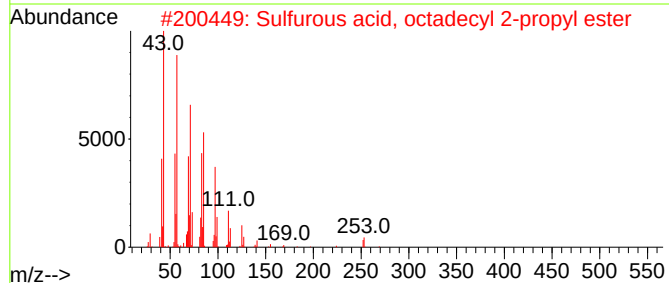
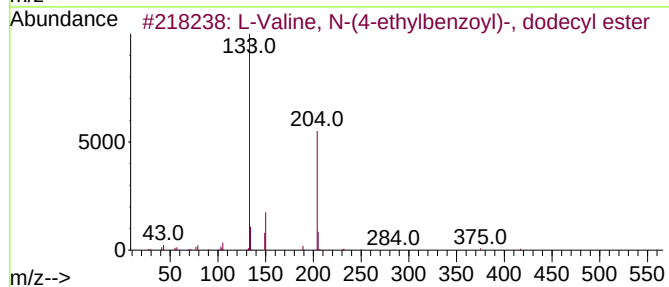
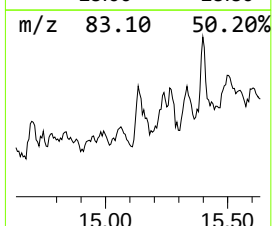
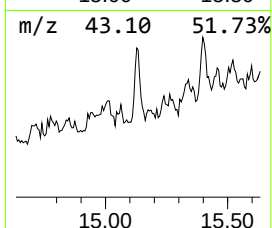
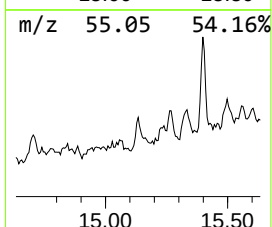
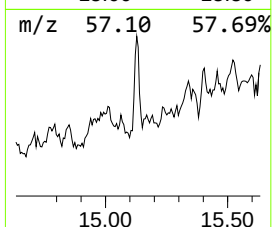
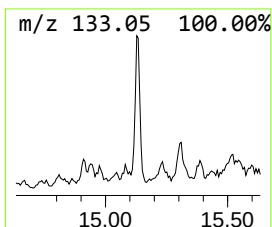
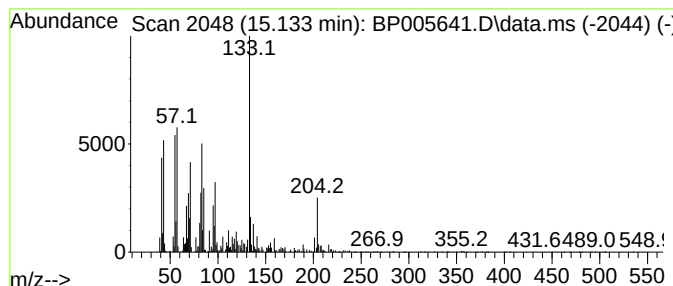
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Peak Number 5 unknown15.13 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.133	2.01 ng	288844	Acenaphthene-d10	14.604

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			L-Valine, N-(4-ethylbenzoyl)-, d...	417	C26H43NO3	1000346-63-5	27
2			Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	25
3			Oxalic acid, isobutyl pentadecyl...	356	C21H40O4	1000309-38-0	22
4			4-Ethylbenzoic acid, oct-3-en-2-...	260	C17H24O2	1000292-54-4	22
5			Undecane, 5-cyclohexyl-	238	C17H34	013151-80-9	18



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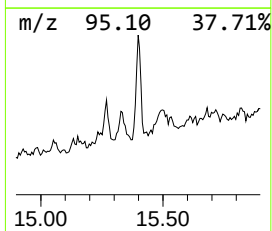
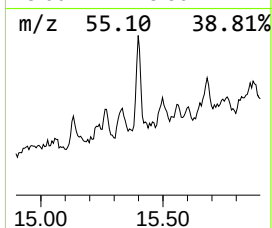
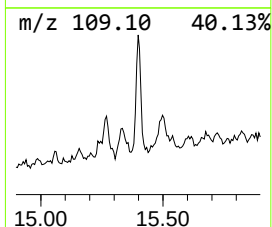
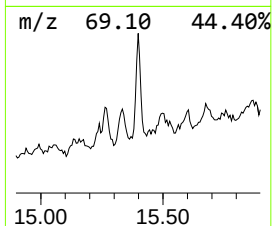
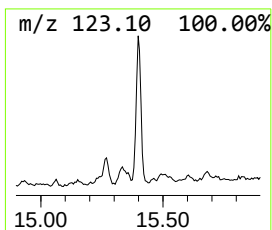
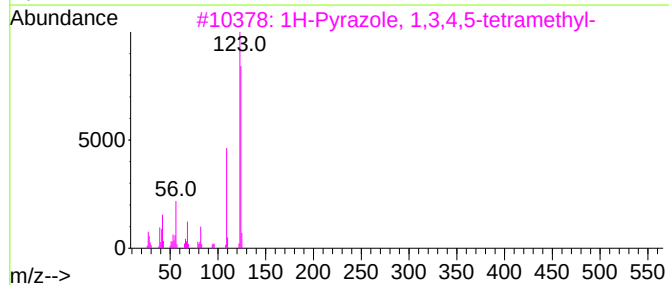
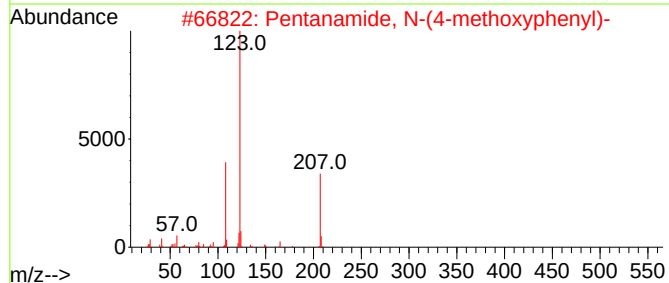
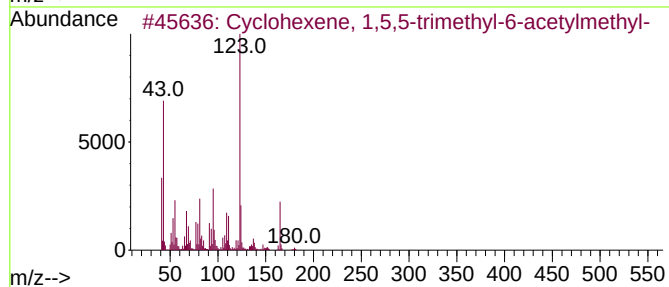
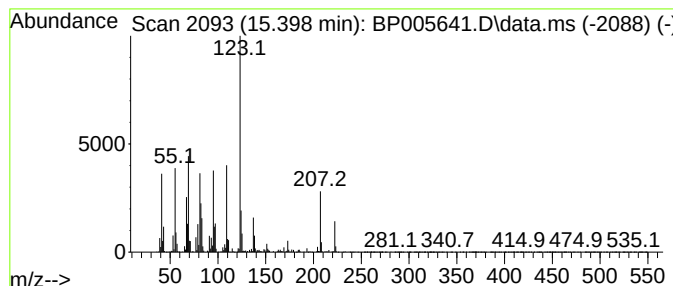
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Cyclohexene, 1,5,5-trimethy... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.398	6.10 ng	876084	Acenaphthene-d10	14.604

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclohexene, 1,5,5-trimethyl-6-a...	180	C12H20O	211563-96-1	50
2		Pentanamide, N-(4-methoxyphenyl)-	207	C12H17NO2	1000306-89-3	43
3		1H-Pyrazole, 1,3,4,5-tetramethyl-	124	C7H12N2	001073-20-7	43
4		4-Fluorobenzoic acid, 5-pentadec...	350	C22H35FO2	1000280-68-6	38
5		2-Fluorobenzoic acid, 2-ethylcyc...	250	C15H19FO2	1000278-98-1	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP052821\
Data File : BP005641.D
Acq On : 28 May 2021 16:22
Operator : CG/JU
Sample : M2560-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
S1-COMP-A-B-C-D

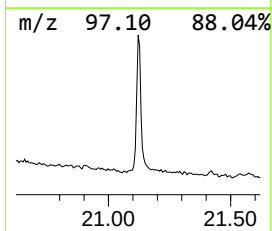
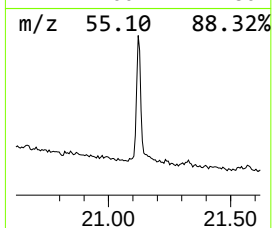
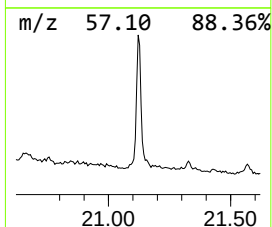
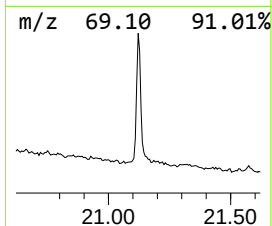
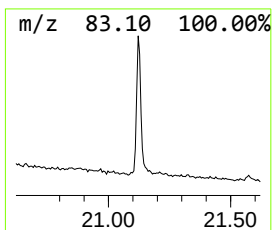
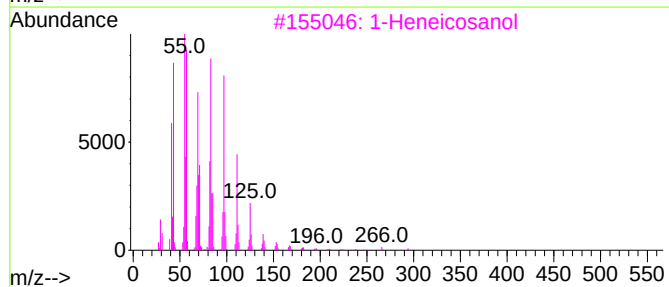
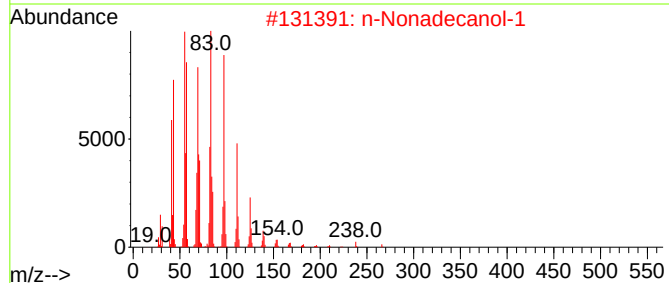
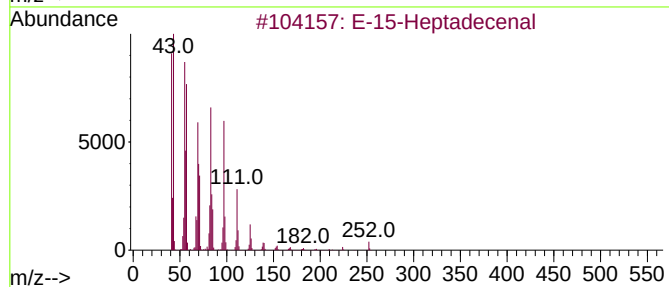
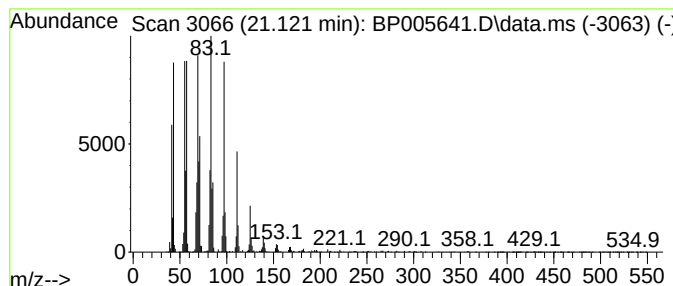
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 E-15-Heptadecenal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.121	8.31 ng	1553440	Chrysene-d12	21.416

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			E-15-Heptadecenal	252	C17H32O	1000130-97-9	98
2			n-Nonadecanol-1	284	C19H40O	001454-84-8	94
3			1-Heneicosanol	312	C21H44O	015594-90-8	94
4			Behenic alcohol	326	C22H46O	000661-19-8	94
5			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP052821\
Data File : BP005641.D
Acq On : 28 May 2021 16:22
Operator : CG/JU
Sample : M2560-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
S1-COMP-A-B-C-D

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP052721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	3.116	29.3	ng	1921660	1	7.987	1313260	20.0
unknown3.15	3.158	2.6	ng	167835	1	7.987	1313260	20.0
2-Pentanone, 4-...	5.081	3.1	ng	203788	1	7.987	1313260	20.0
1-(2-Hydroxyeth...	14.445	4.5	ng	640741	3	14.604	2872760	20.0
unknown15.13	15.133	2.0	ng	288844	3	14.604	2872760	20.0
Cyclohexene, 1,...	15.398	6.1	ng	876084	3	14.604	2872760	20.0
E-15-Heptadecenal	21.121	8.3	ng	1553440	5	21.416	3737810	20.0