

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM120321\
 Data File : BM033300.D
 Acq On : 03 Dec 2021 23:25
 Operator : CG/JU
 Sample : M4917-10
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 MW-26

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_M\Methods\8270-BM112421.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM033300.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.660	50	55	63	rBV2	86125	153851	1.79%	0.367%
2	5.049	285	291	297	rBV	216734	317387	3.68%	0.757%
3	5.513	363	370	387	rVB	1671770	2546171	29.55%	6.075%
4	6.119	467	473	481	rVB	62443	100626	1.17%	0.240%
5	7.107	634	641	653	rBV	1074489	1746112	20.27%	4.166%
6	7.925	772	780	788	rBV	535657	869947	10.10%	2.076%
7	9.090	970	978	987	rBV	2015972	3397271	39.43%	8.106%
8	10.495	1210	1217	1233	rBV	486157	809923	9.40%	1.932%
9	10.725	1246	1256	1267	rBV	669193	1176020	13.65%	2.806%
10	13.172	1665	1672	1681	rBV	4282422	6391576	74.19%	15.250%
11	14.354	1867	1873	1878	rBV	88766	149649	1.74%	0.357%
12	14.548	1899	1906	1913	rBV	949458	1425266	16.54%	3.401%
13	16.036	2152	2159	2169	rBV	3225291	4655470	54.04%	11.108%
14	17.289	2366	2372	2379	rBV	1134167	1633029	18.95%	3.896%
15	18.171	2517	2522	2530	rBV	80092	148994	1.73%	0.356%
16	19.112	2679	2682	2688	rVB	98853	106017	1.23%	0.253%
17	19.718	2779	2785	2803	rBV	2286262	3717224	43.15%	8.869%
18	19.895	2810	2815	2823	rVB	6632585	8615510	100.00%	20.557%
19	21.148	3025	3028	3035	rVB3	126582	171744	1.99%	0.410%
20	21.224	3038	3041	3045	rBV	82970	105390	1.22%	0.251%
21	21.448	3074	3079	3084	rBV	1401576	1787353	20.75%	4.265%
22	23.777	3469	3475	3488	rVB	954116	1886327	21.89%	4.501%

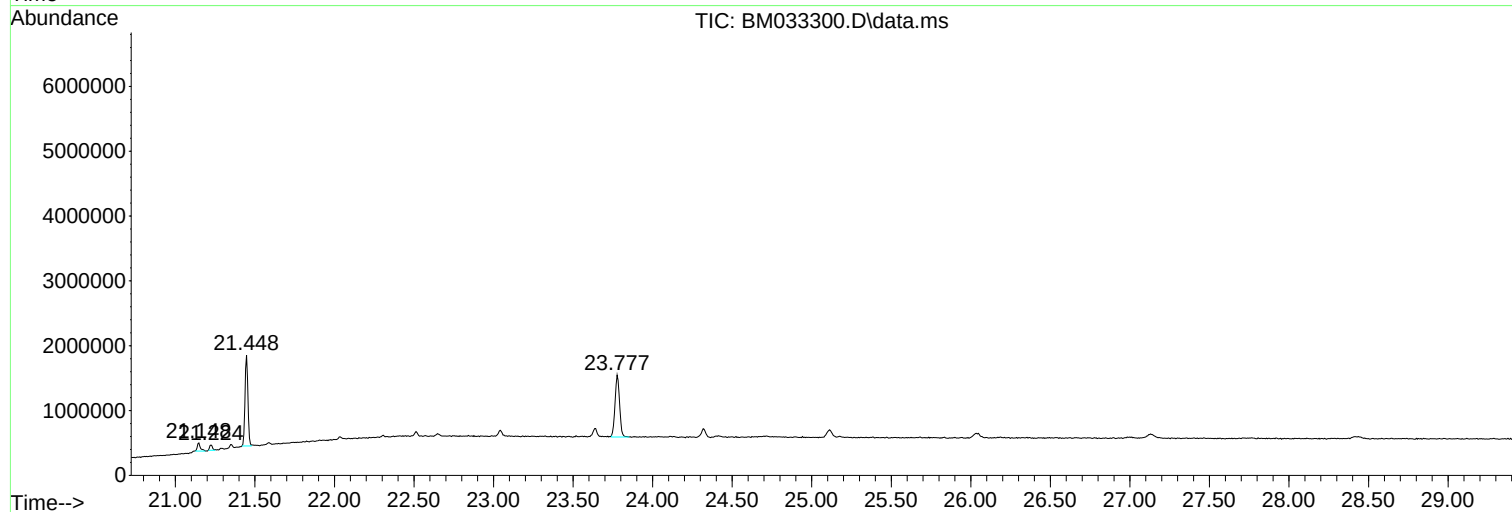
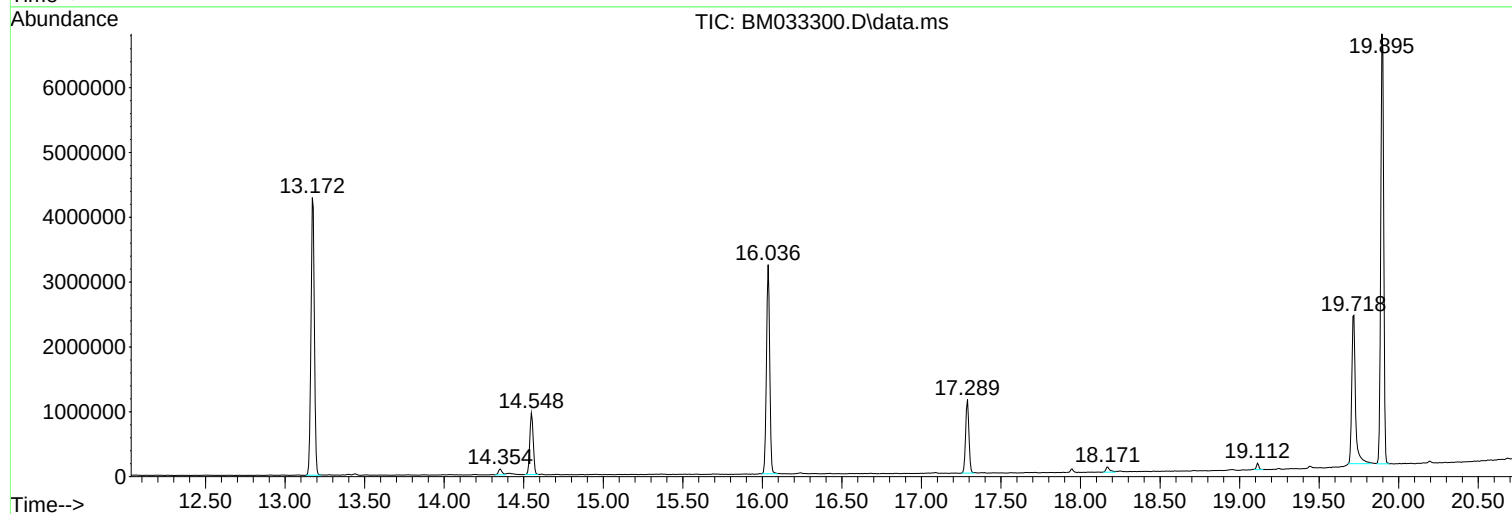
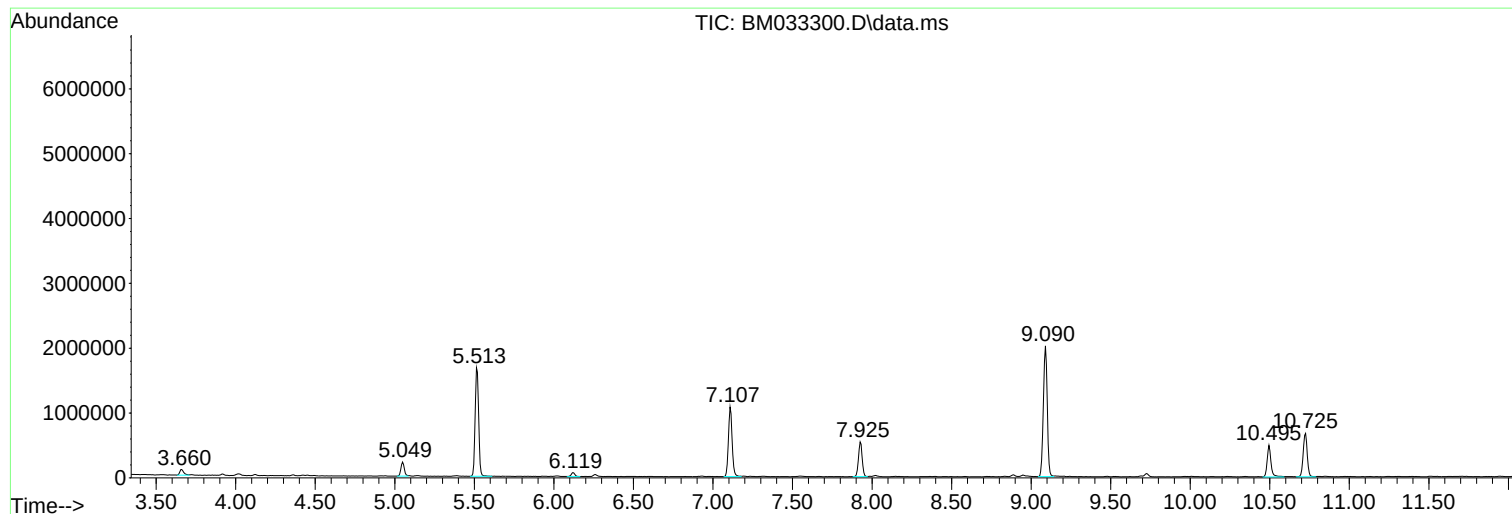
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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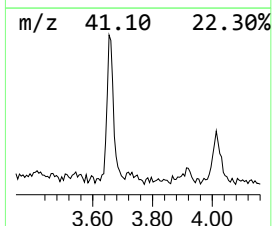
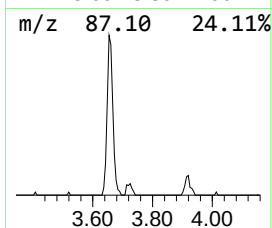
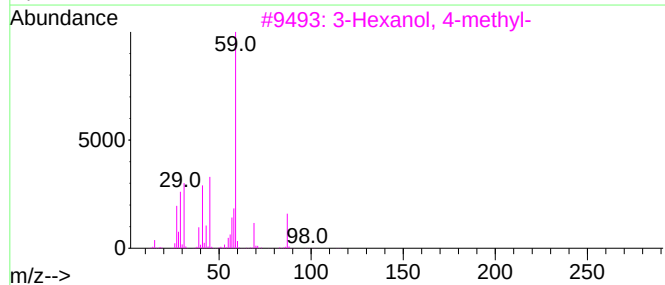
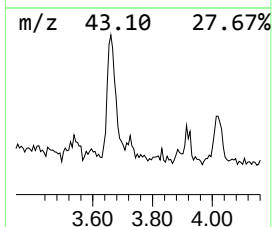
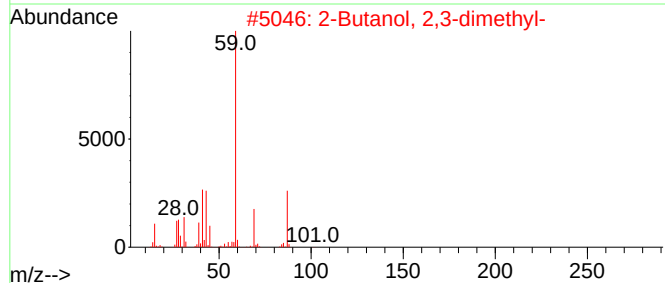
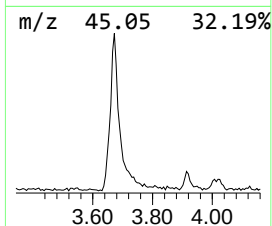
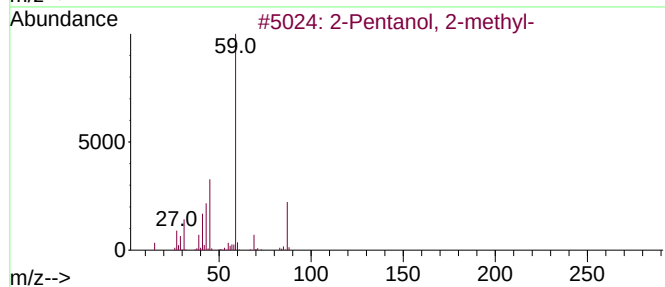
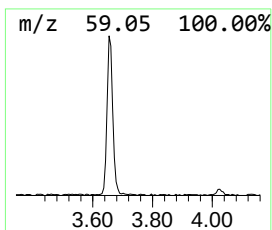
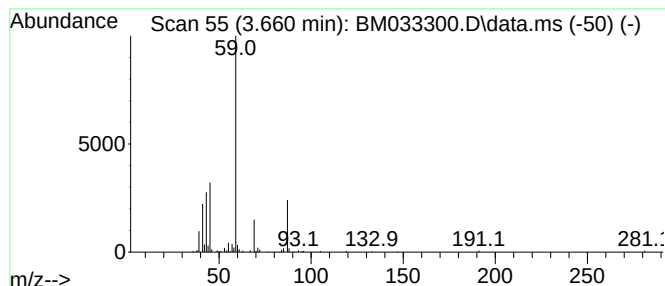
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanol, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.660	3.54 ng	153851	1,4-Dichlorobenzene-d4	7.925

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanol, 2-methyl-	102	C6H14O	000590-36-3	78	
2	2-Butanol, 2,3-dimethyl-	102	C6H14O	000594-60-5	72	
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	64	
4	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	53	
5	3-Pentanol, 2,2-dimethyl-	116	C7H16O	003970-62-5	43	



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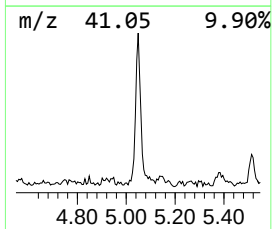
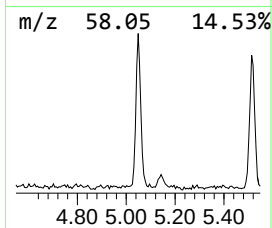
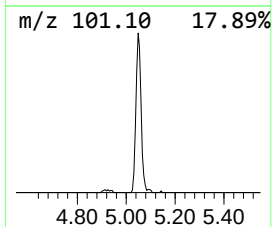
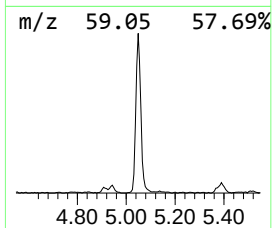
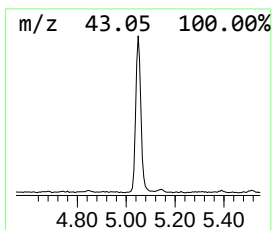
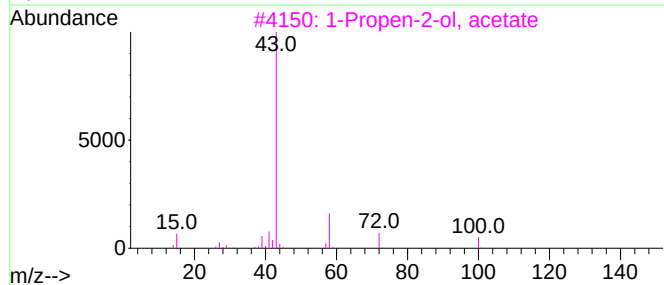
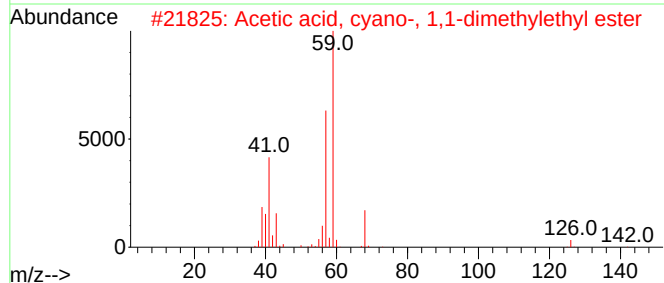
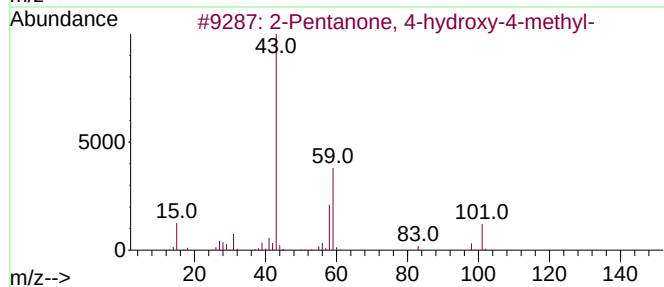
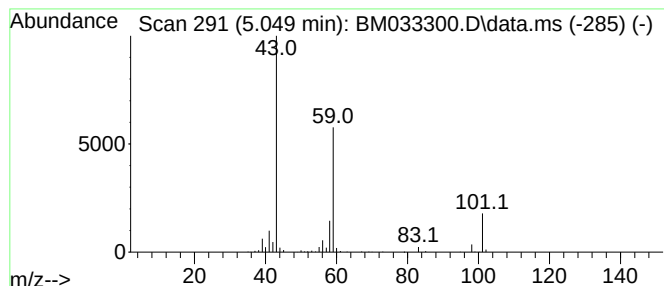
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.049	7.30 ng	317387	1,4-Dichlorobenzene-d4	7.925

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, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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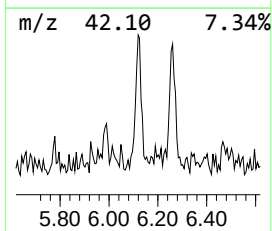
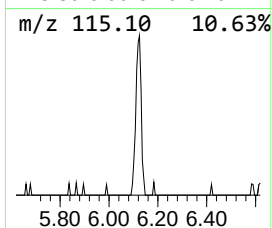
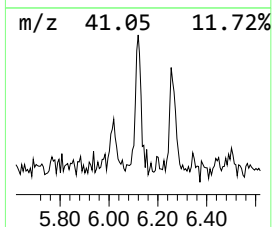
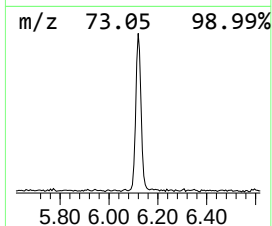
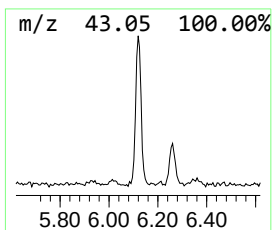
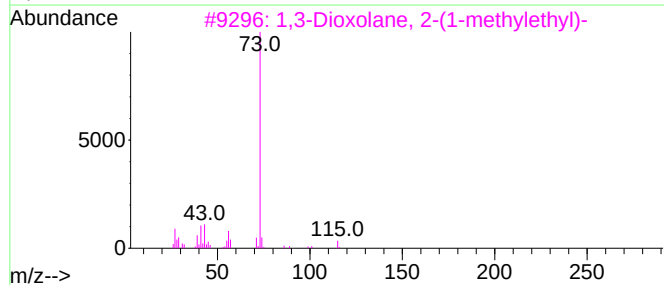
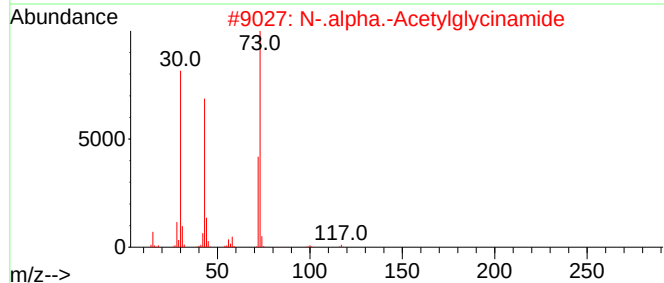
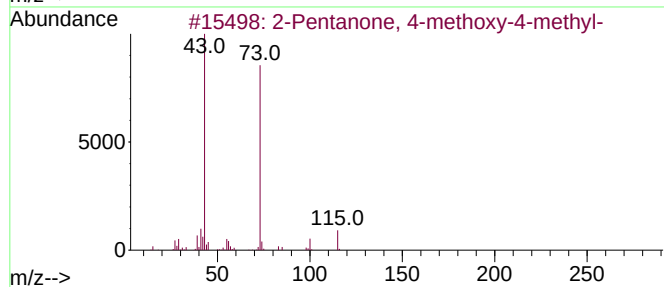
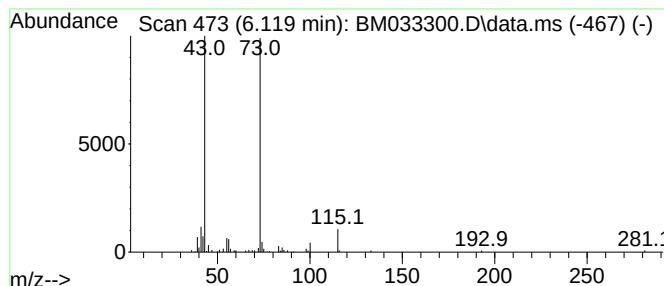
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Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.119	2.31 ng	100626	1,4-Dichlorobenzene-d4	7.925

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	64
2		N-.alpha.-Acetylglycinamide	116	C4H8N2O2	002620-63-5	38
3		1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	27
4		Butane, 2-methoxy-2,3,3-trimethyl-	130	C8H18O	027705-21-1	23
5		Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	12



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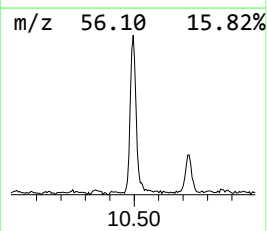
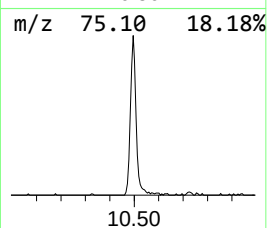
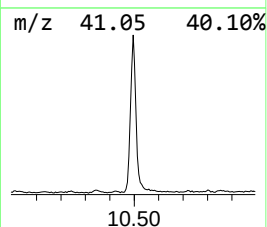
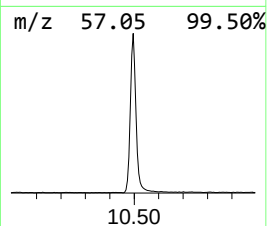
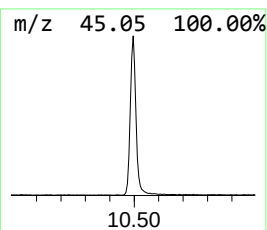
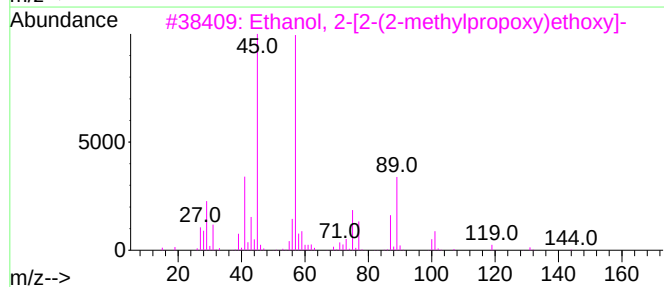
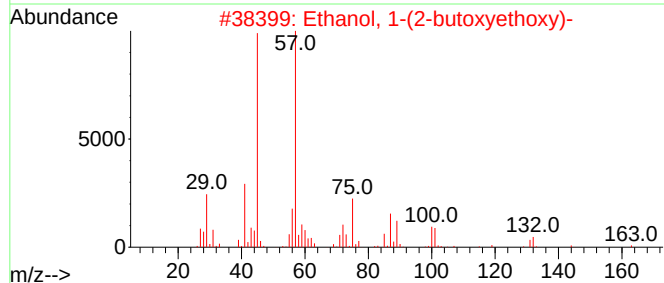
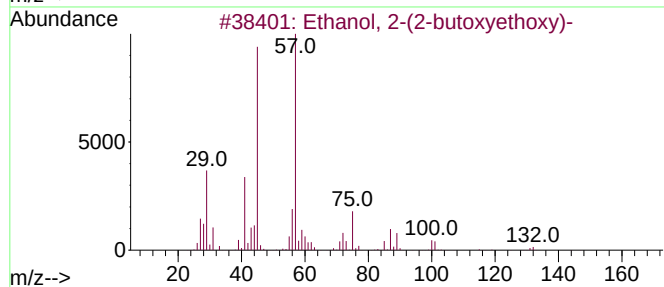
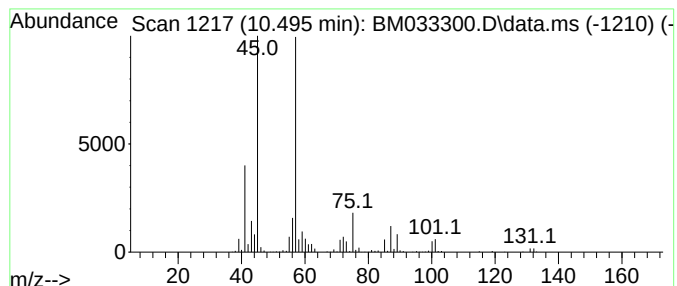
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Peak Number 4 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.495	13.77 ng	809923	Naphthalene-d8	10.725

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	90
3			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	78
4			Di-sec-Butyl ether	130	C8H18O	006863-58-7	53
5			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	50



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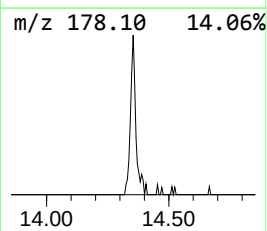
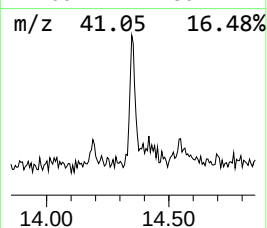
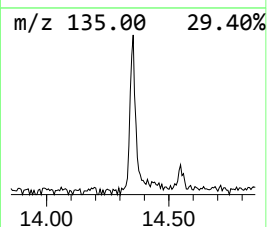
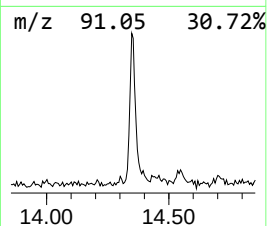
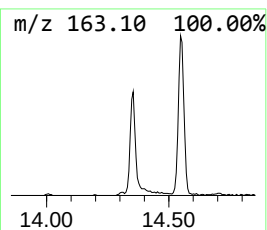
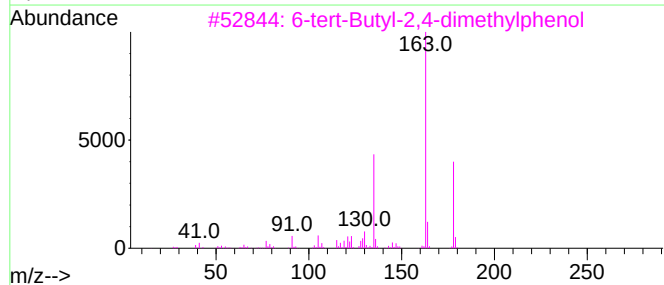
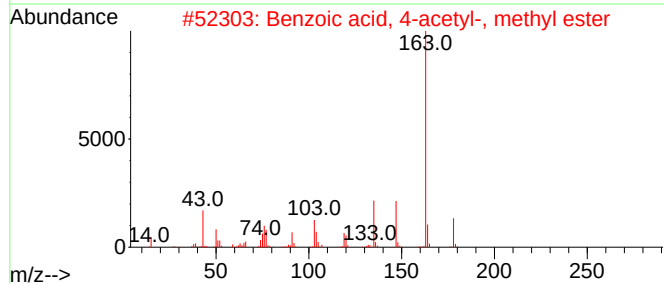
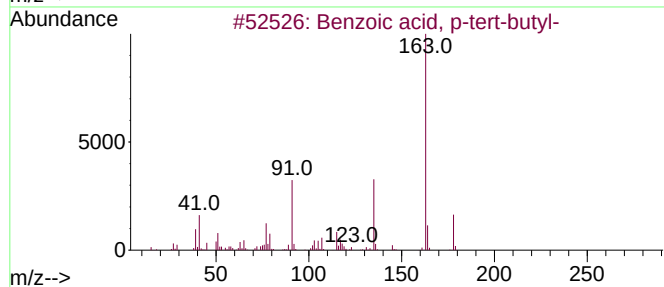
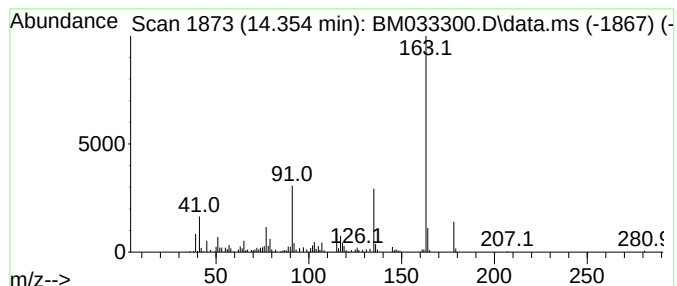
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Peak Number 5 Benzoic acid, p-tert-butyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.354	2.10 ng	149649	Acenaphthene-d10	14.548

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoic acid, p-tert-butyl-	178	C11H14O2	000098-73-7	96
2			Benzoic acid, 4-acetyl-, methyl ...	178	C10H10O3	003609-53-8	80
3			6-tert-Butyl-2,4-dimethylphenol	178	C12H18O	001879-09-0	74
4			Benzaldehyde, 5-(1,1-dimethyleth...	178	C11H14O2	002725-53-3	64
5			5-Fluoro-8-quinolinol	163	C9H6FNO	000387-97-3	64



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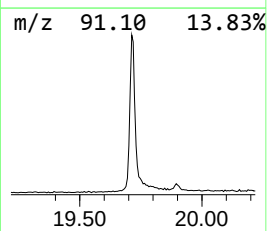
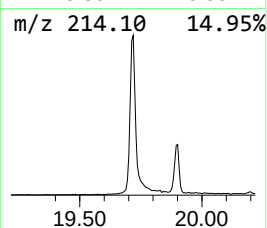
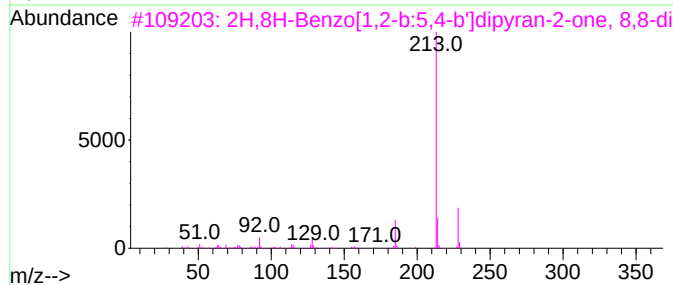
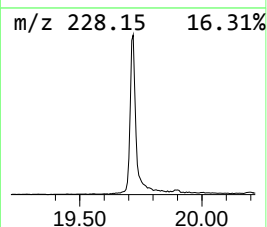
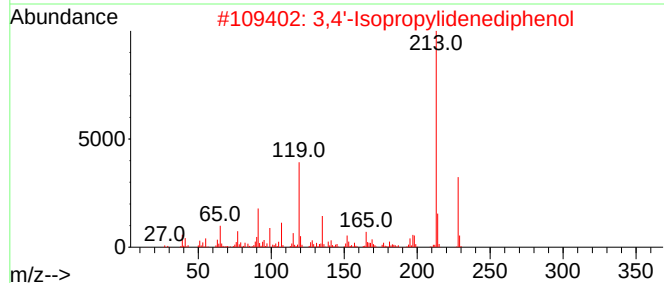
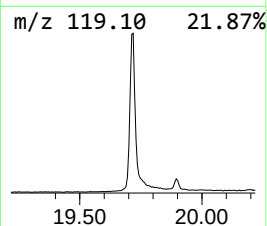
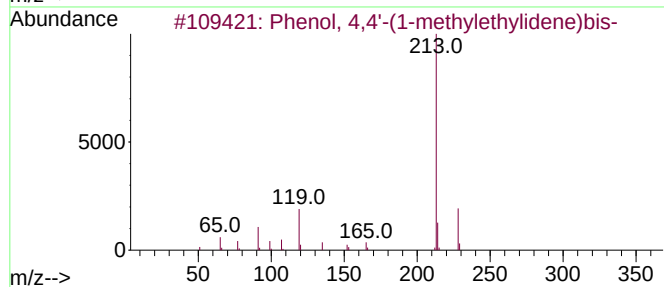
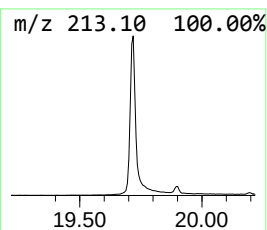
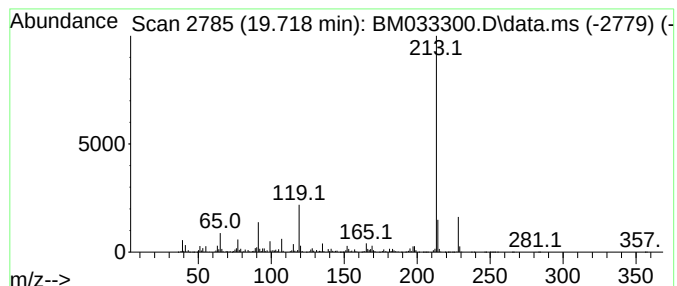
Instrument :
BNA_M
ClientSampleId :
MW-26

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM112421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Phenol, 4,4'-(1-methylethyl... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.718	41.59 ng	3717220	Chrysene-d12	21.448	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	98
2	3,4'-Isopropylidenediphenol	228	C15H16O2	046765-25-7	78
3	2H,8H-Benzo[1,2-b:5,4-b']dipyran...	228	C14H12O3	000553-19-5	52
4	Pyridine, 2-(5-trifluoromethyl-3...	213	C9H6F3N3	003974-71-8	50
5	3-Cyano-4-ethyl-6-methylcoumarin	213	C13H11NO2	025937-11-5	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM120321\
Data File : BM033300.D
Acq On : 03 Dec 2021 23:25
Operator : CG/JU
Sample : M4917-10
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MW-26

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM112421.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
2-Pentanol, 2-m...	3.660	3.5	ng	153851	1	7.925	869947	20.0
2-Pentanone, 4-...	5.049	7.3	ng	317387	1	7.925	869947	20.0
2-Pentanone, 4-...	6.119	2.3	ng	100626	1	7.925	869947	20.0
Ethanol, 2-(2-b...	10.495	13.8	ng	809923	2	10.725	1176020	20.0
Benzoic acid, p...	14.354	2.1	ng	149649	3	14.548	1425270	20.0
Phenol, 4,4'-(1...	19.718	41.6	ng	3717220	5	21.448	1787350	20.0