

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM091923\
 Data File : BM041920.D
 Acq On : 20 Sep 2023 01:41
 Operator : MA/JU
 Sample : 04299-10
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 TWP-01

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-BM091823.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM041920.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.440	207	213	230	rVB	2706599	3570101	26.39%	4.016%
2	5.057	309	318	326	rBV	1203912	1657740	12.25%	1.865%
3	5.499	386	393	403	rBV	2566505	3593828	26.56%	4.042%
4	7.104	658	666	678	rBV	2268737	3563608	26.34%	4.008%
5	7.546	736	741	751	rVB	103226	170766	1.26%	0.192%
6	7.963	804	812	823	rBV	1182733	2012932	14.88%	2.264%
7	9.151	1004	1014	1028	rBV	3027920	5084384	37.58%	5.719%
8	10.781	1283	1291	1297	rBV	1575627	2708648	20.02%	3.047%
9	13.227	1701	1707	1719	rVB	7340142	10744117	79.41%	12.085%
10	14.610	1935	1942	1949	rVB	2445675	3643326	26.93%	4.098%
11	15.410	2071	2078	2084	rVB	154002	219239	1.62%	0.247%
12	16.098	2188	2195	2208	rBV	4058086	5799723	42.86%	6.524%
13	17.357	2402	2409	2422	rVB	2971663	4370875	32.30%	4.917%
14	18.210	2548	2554	2567	rBV	2288984	3343969	24.71%	3.761%
15	19.445	2760	2764	2766	rBV2	105968	149398	1.10%	0.168%
16	19.480	2766	2770	2777	rVB	514129	685544	5.07%	0.771%
17	19.621	2791	2794	2799	rBV	181333	193363	1.43%	0.218%
18	19.686	2802	2805	2811	rVB	186579	208737	1.54%	0.235%
19	19.968	2847	2853	2858	rBV	11197939	13530350	100.00%	15.219%
20	20.221	2892	2896	2900	rVB	277954	338429	2.50%	0.381%
21	20.715	2977	2980	2983	rBV	283561	271839	2.01%	0.306%
22	21.192	3056	3061	3071	rBV	2128375	2950957	21.81%	3.319%
23	21.392	3092	3095	3099	rVB	461859	508401	3.76%	0.572%
24	21.533	3114	3119	3124	rVB	3301797	4427288	32.72%	4.980%
25	21.615	3131	3133	3137	rVB	255504	256735	1.90%	0.289%
26	22.074	3208	3211	3214	rVV	237455	256837	1.90%	0.289%
27	22.115	3215	3218	3224	rVB3	179601	265482	1.96%	0.299%
28	22.362	3256	3260	3267	rBV	358746	490143	3.62%	0.551%
29	22.562	3291	3294	3301	rVB2	234666	297042	2.20%	0.334%
30	23.103	3383	3386	3395	rVB	239136	390567	2.89%	0.439%
31	23.944	3523	3529	3541	rVB	1999968	4042972	29.88%	4.548%
32	26.362	3930	3940	3965	rBV2	2918816	9154495	67.66%	10.297%

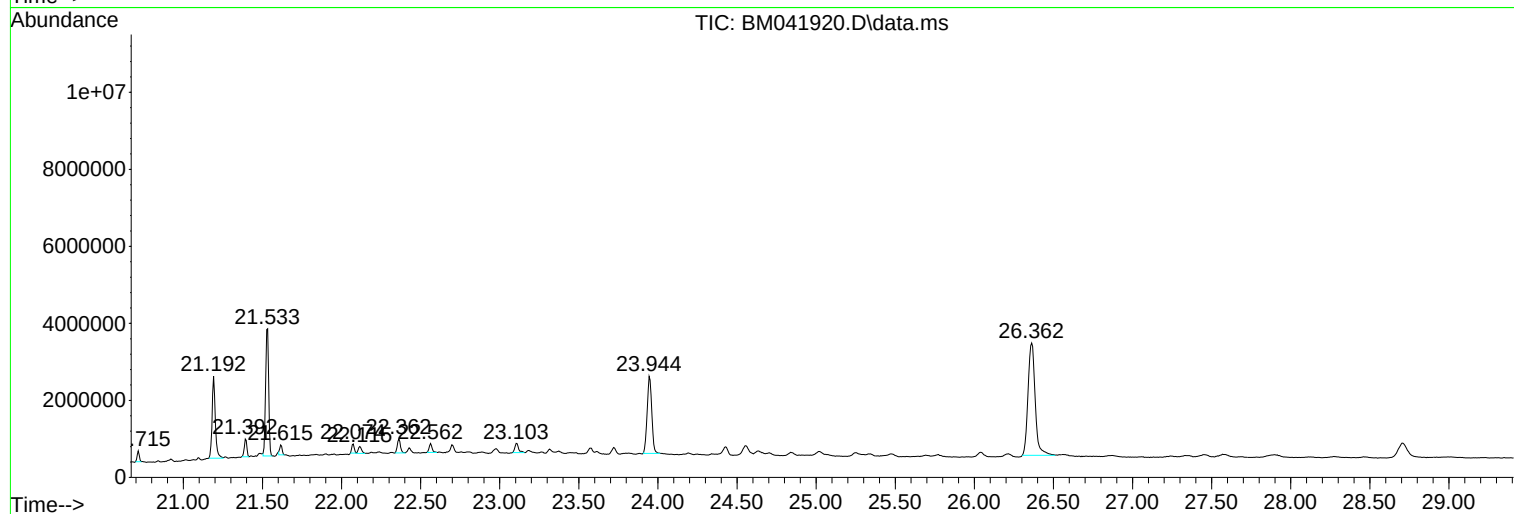
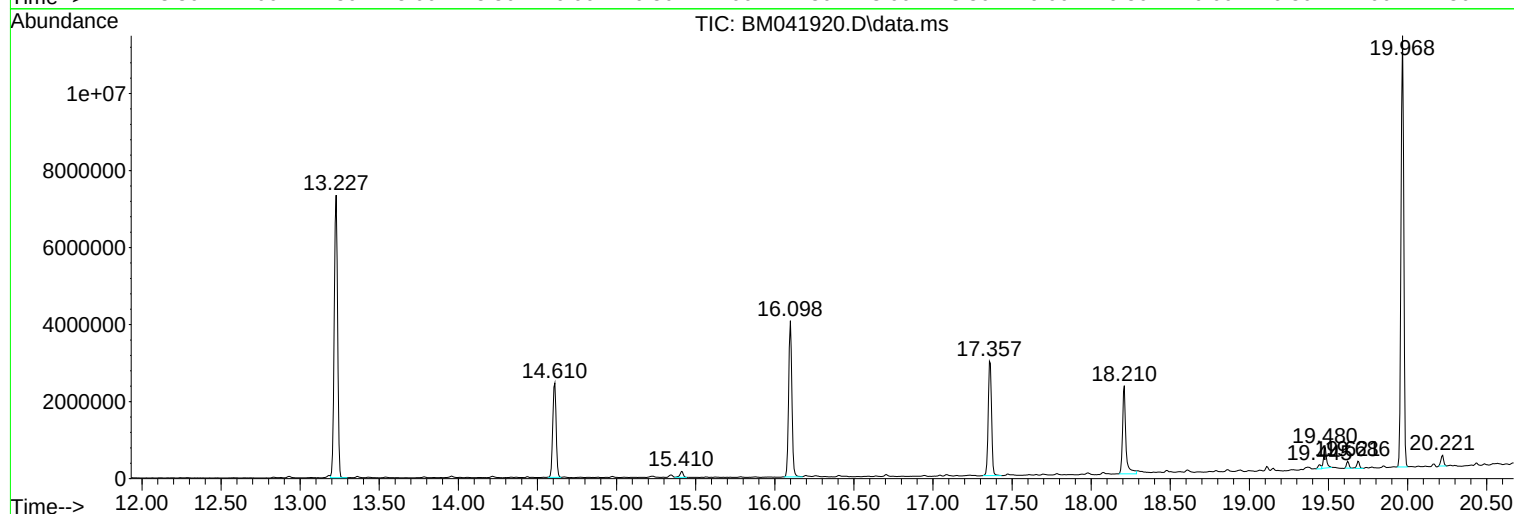
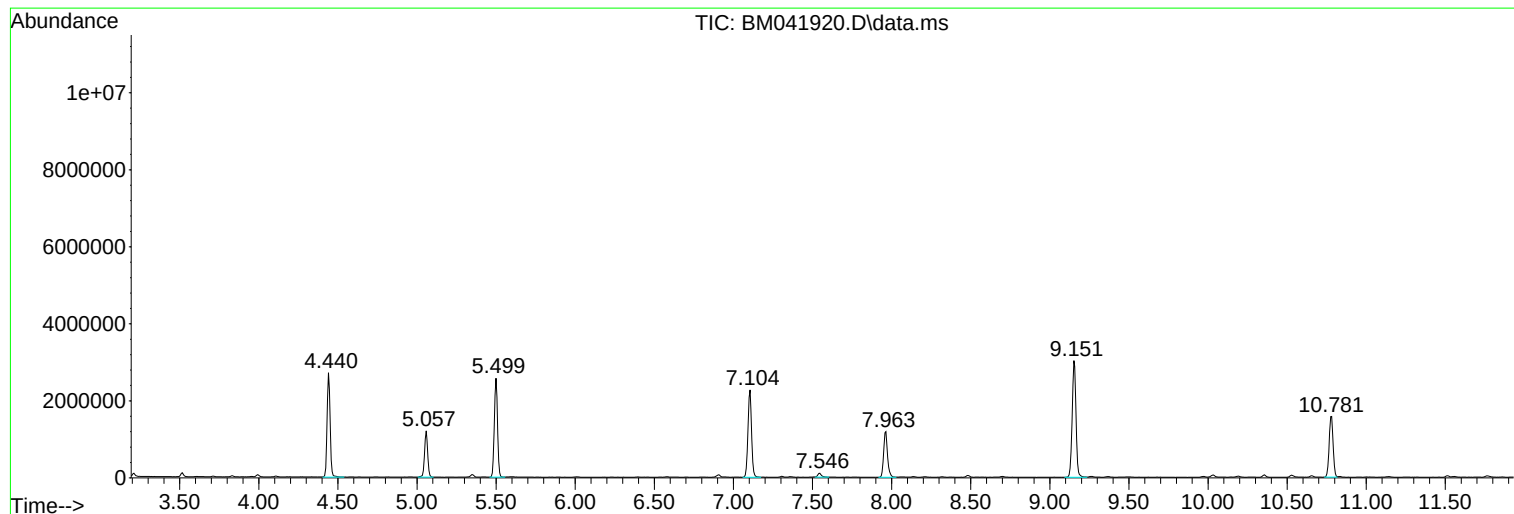
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM091823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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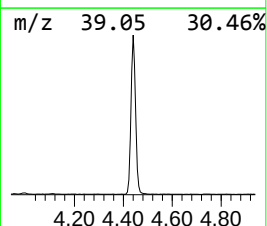
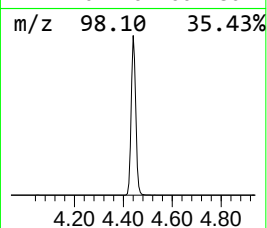
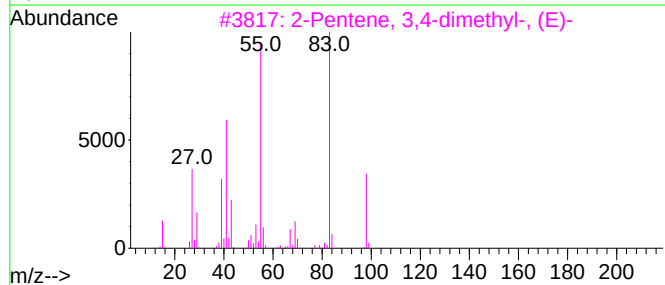
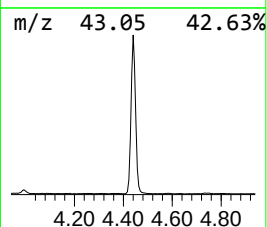
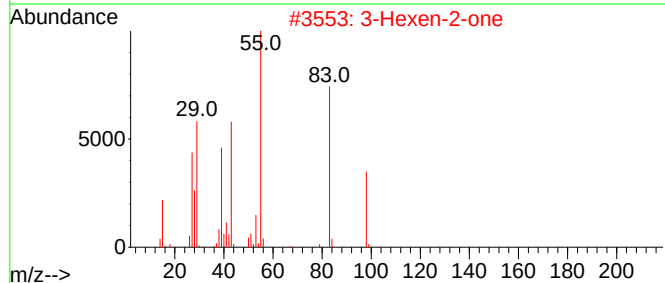
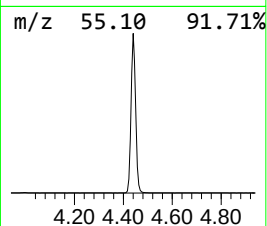
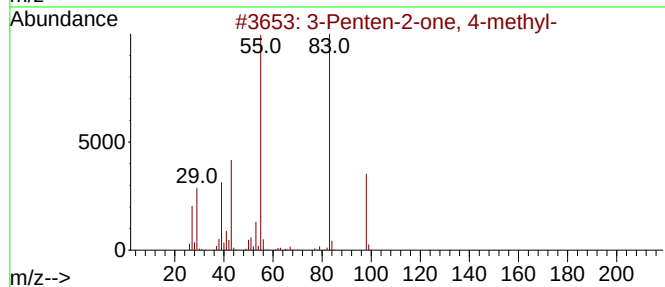
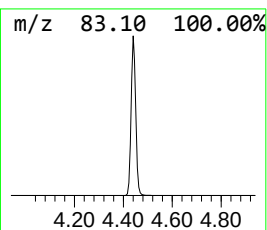
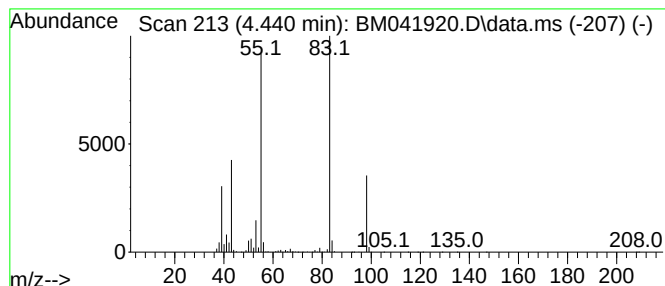
Instrument :
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD			R.T.
4.440	35.47 ng	3570100	1,4-Dichlorobenzene-d4			7.963
Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-		98	C6H10O	000141-79-7	95
2	3-Hexen-2-one		98	C6H10O	000763-93-9	91
3	2-Pentene, 3,4-dimethyl-, (E)-		98	C7H14	004914-92-5	90
4	2-Pentene, 3,4-dimethyl-, (Z)-		98	C7H14	004914-91-4	86
5	2-Pentene, 2,4-dimethyl-		98	C7H14	000625-65-0	80



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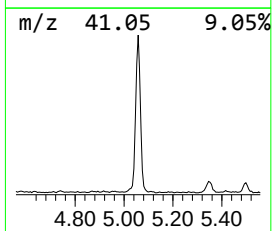
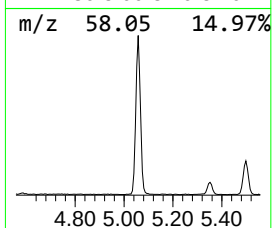
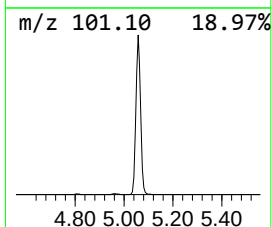
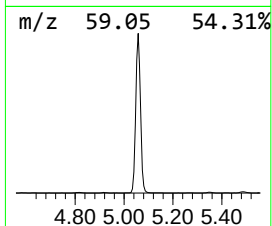
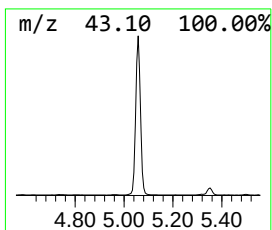
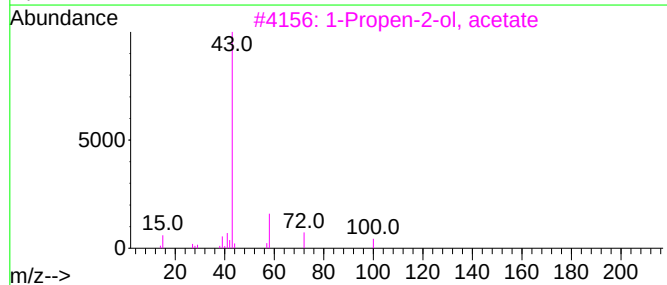
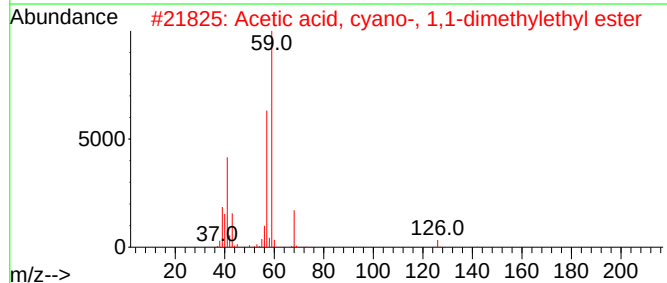
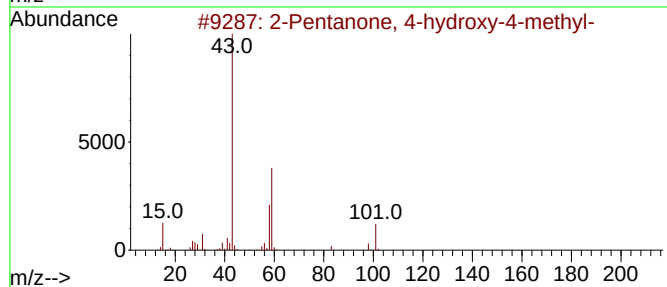
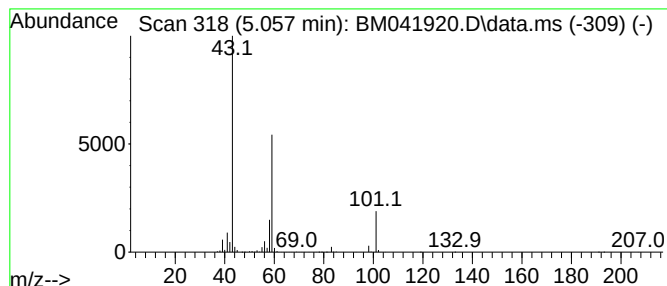
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM091823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.057	16.47 ng	1657740	1,4-Dichlorobenzene-d4	7.963

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50	
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25	
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12	
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9	
5	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9	



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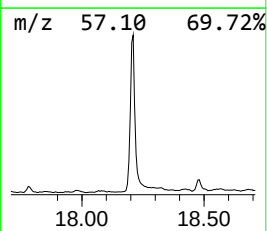
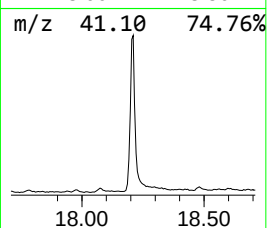
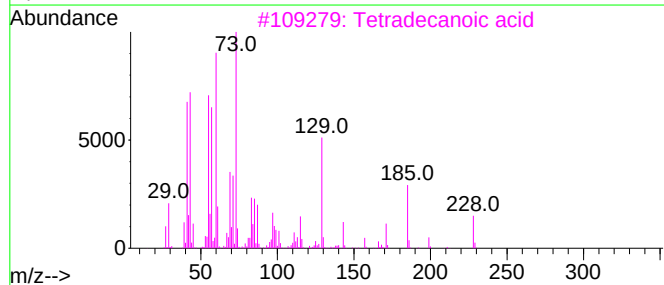
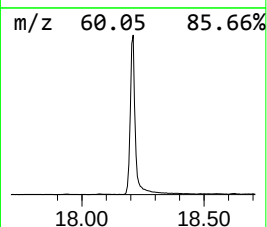
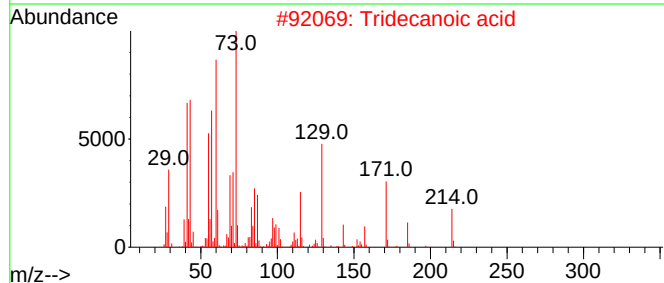
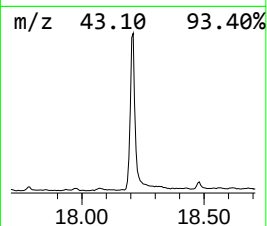
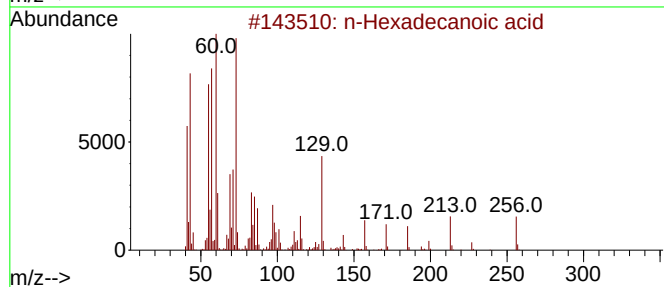
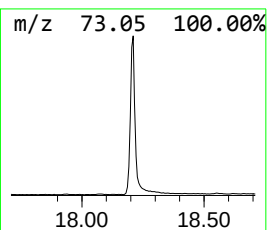
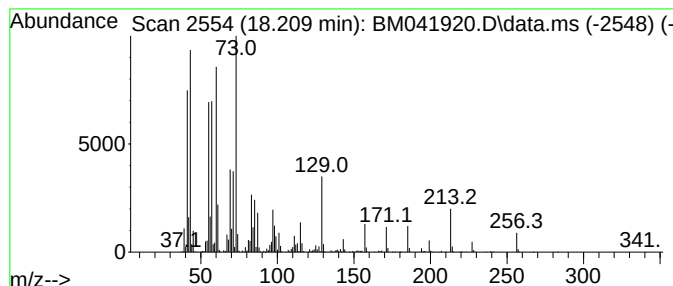
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.209	15.30 ng	3343970	Phenanthrene-d10	17.357

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	92
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	90
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5			Dodecanoic acid	200	C12H24O2	000143-07-7	58



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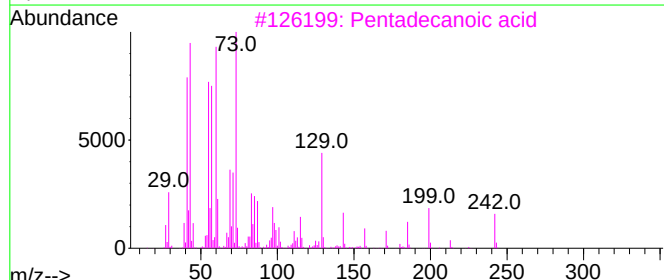
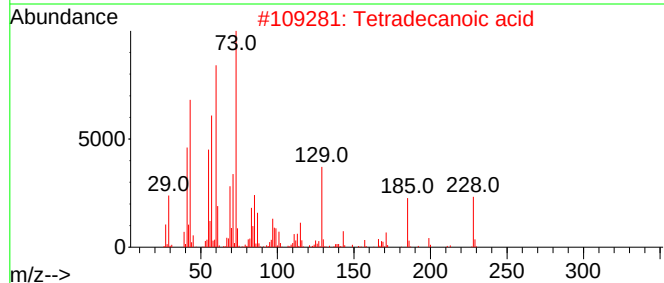
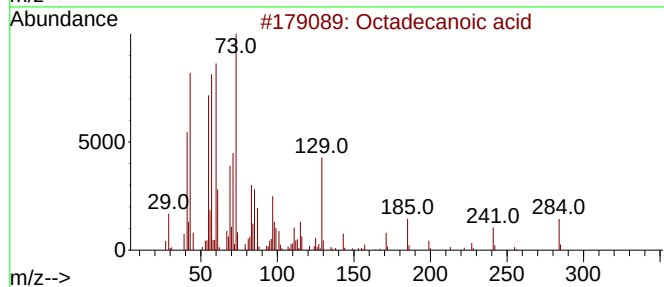
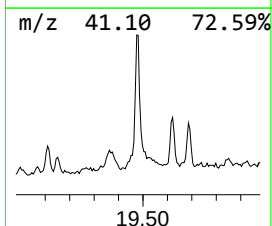
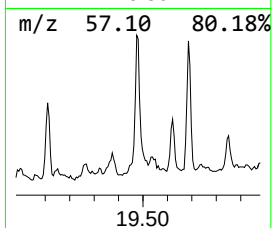
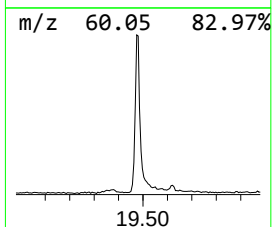
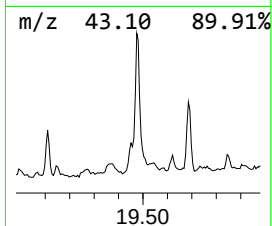
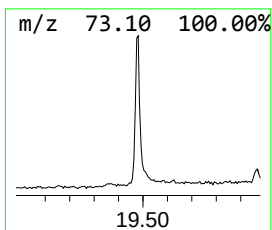
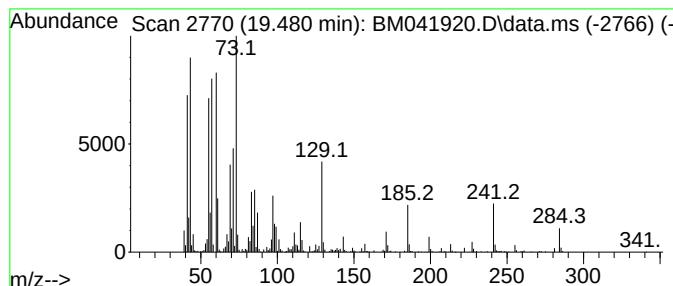
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.480	3.10 ng	685544	Chrysene-d12	21.533

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	76
4			Tridecanoic acid	214	C13H26O2	000638-53-9	64
5			n-Decanoic acid	172	C10H20O2	000334-48-5	60



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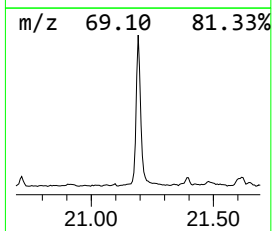
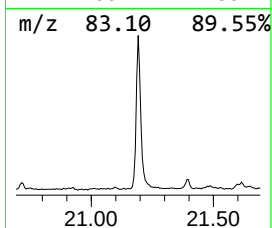
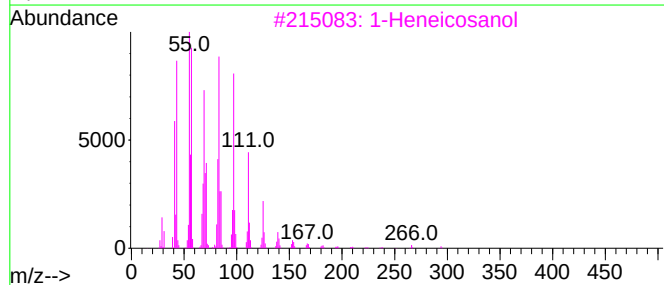
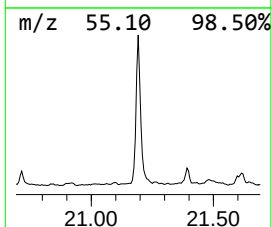
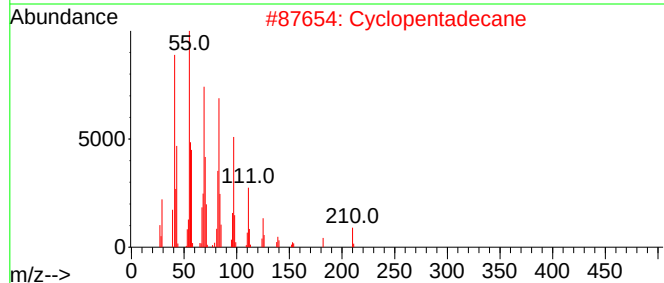
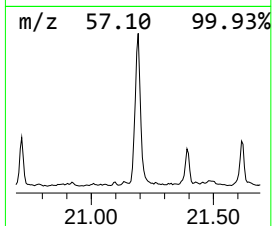
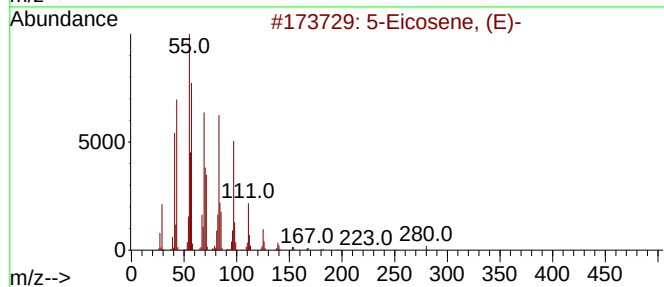
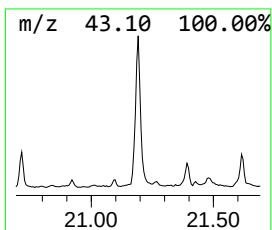
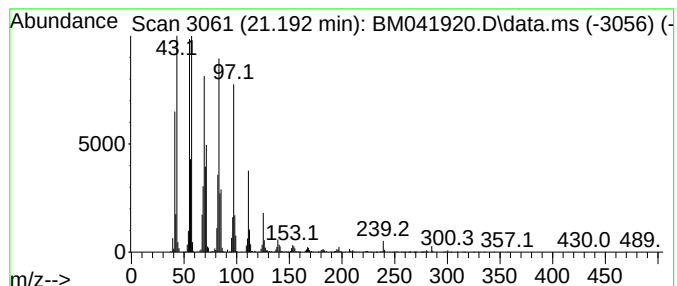
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 5-Eicosene, (E)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.192	13.33 ng	2950960	Chrysene-d12	21.533

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Eicosene, (E)-	280	C20H40	074685-30-6	99
2			Cyclopentadecane	210	C15H30	000295-48-7	97
3			1-Heneicosanol	312	C21H44O	015594-90-8	95
4			n-Tetracosanol-1	354	C24H50O	000506-51-4	94
5			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94



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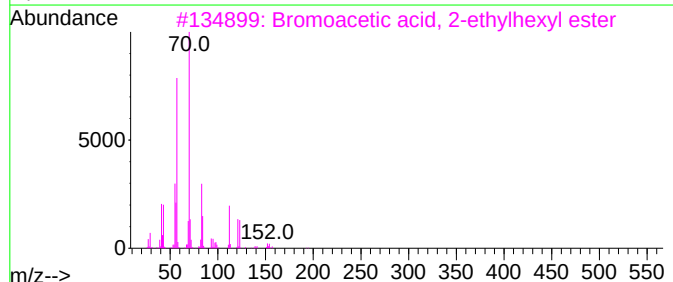
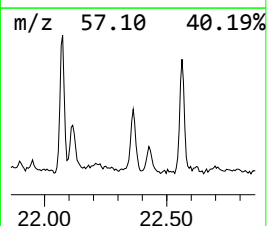
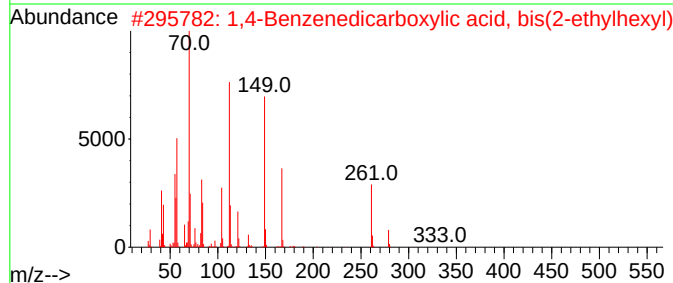
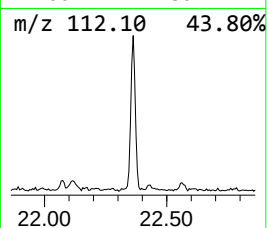
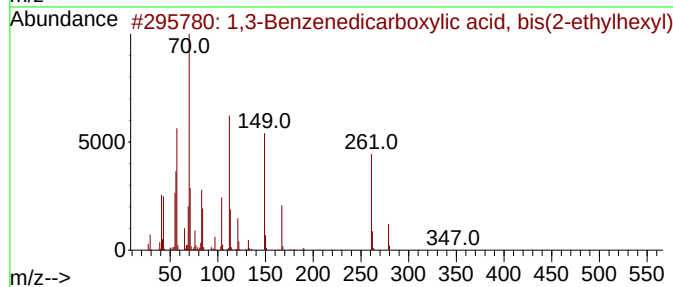
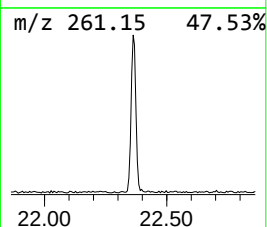
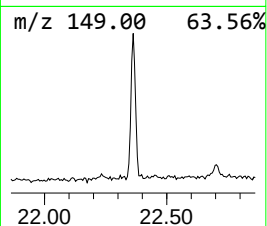
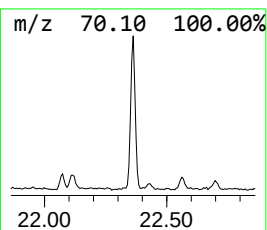
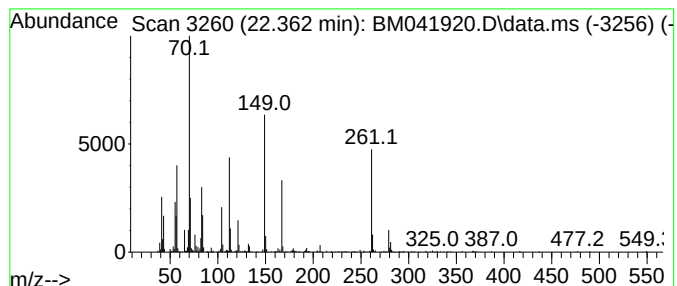
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1,3-Benzenedicarboxylic aci... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.362	2.21 ng	490143	Chrysene-d12	21.533

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	83
2			1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	68
3			Bromoacetic acid, 2-ethylhexyl e...	250	C10H19BrO2	068144-73-0	22
4			4-Methyl-N-(4-nitrophenyl)pipera...	294	C13H18N4O2S	1000488-00-4	14
5			9-(2',2'-Dimethylpropanoilhydraz...	576	C30H42Cl2N4O3	1000111-04-6	14



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM091923\
Data File : BM041920.D
Acq On : 20 Sep 2023 01:41
Operator : MA/JU
Sample : 04299-10
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TWP-01

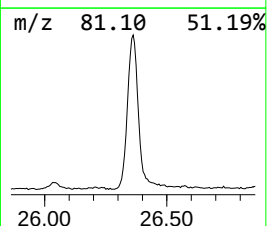
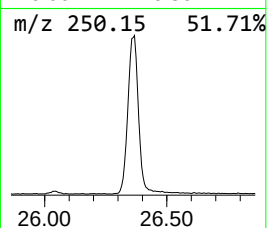
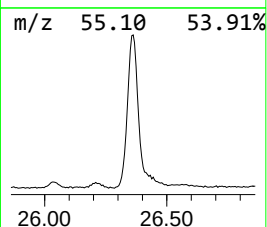
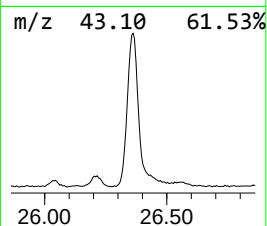
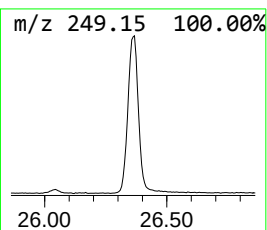
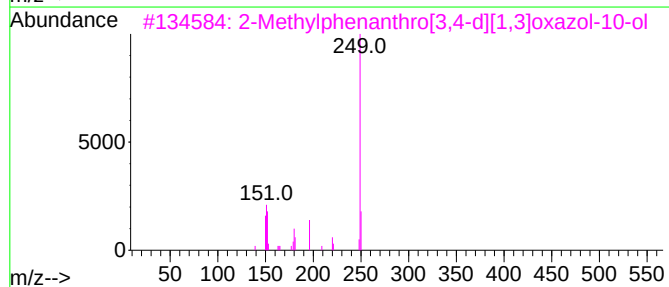
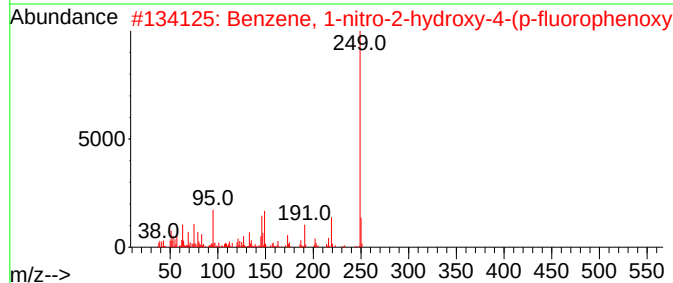
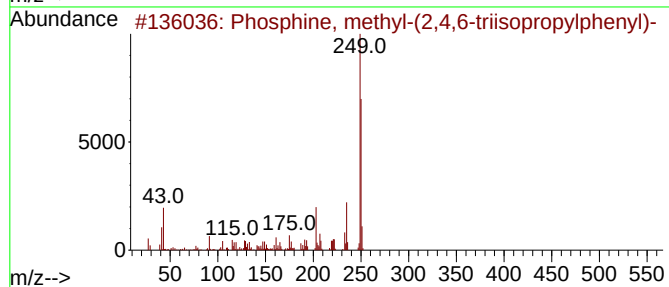
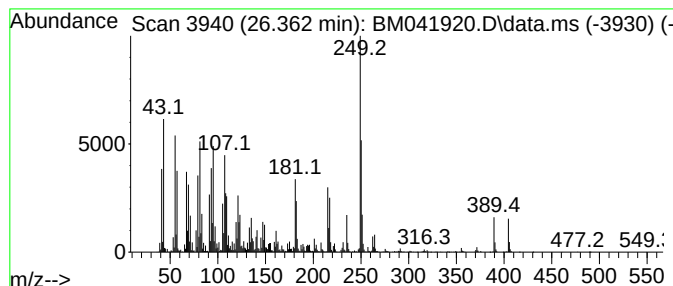
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown26.362 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.362	45.29 ng	9154500	Perylene-d12	23.944

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phosphine, methyl-(2,4,6-triisop...	250	C16H27P	158748-69-7	38
2			Benzene, 1-nitro-2-hydroxy-4-(p-...	249	C12H8FN04	189214-56-0	38
3			2-Methylphenanthro[3,4-d][1,3]ox...	249	C16H11N02	098033-24-0	35
4			12H-Benzo(b)phenothiazine	249	C16H11NS	000258-08-2	27
5			7H-Benzo(c)phenothiazine	249	C16H11NS	000226-06-2	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM091923\
Data File : BM041920.D
Acq On : 20 Sep 2023 01:41
Operator : MA/JU
Sample : 04299-10
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TWP-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM091823.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
3-Penten-2-one,...	4.440	35.5	ng	3570100	1	7.963	2012930	20.0
2-Pentanone, 4-...	5.057	16.5	ng	1657740	1	7.963	2012930	20.0
n-Hexadecanoic ...	18.209	15.3	ng	3343970	4	17.357	4370880	20.0
Octadecanoic acid	19.480	3.1	ng	685544	5	21.533	4427290	20.0
5-Eicosene, (E)-	21.192	13.3	ng	2950960	5	21.533	4427290	20.0
1,3-Benzenedica...	22.362	2.2	ng	490143	5	21.533	4427290	20.0
unknown26.362	26.362	45.3	ng	9154500	6	23.944	4042970	20.0