

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082324\
 Data File : BM047336.D
 Acq On : 23 Aug 2024 16:48
 Operator : RC/JU
 Sample : P3694-01
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 Kingsland-Driveway

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-BM081024.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM047336.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.263	61	64	80	rVB	114019	180031	2.41%	0.337%
2	4.563	279	285	292	rBV	174888	247054	3.30%	0.462%
3	5.010	355	361	376	rBV	2705937	3928691	52.52%	7.345%
4	6.569	615	626	645	rBV	2415203	4062380	54.30%	7.595%
5	7.351	752	759	770	rBV	1133895	1737391	23.22%	3.248%
6	8.498	947	954	966	rBV	1656771	2666490	35.64%	4.985%
7	9.081	1048	1053	1063	rVB	70782	119057	1.59%	0.223%
8	10.104	1216	1227	1244	rBV	1347607	2271293	30.36%	4.246%
9	10.869	1350	1357	1370	rBV	101870	234565	3.14%	0.439%
10	12.616	1645	1654	1671	rBV	3890769	5847044	78.16%	10.932%
11	14.010	1884	1891	1898	rBV	1983401	2970881	39.71%	5.554%
12	14.074	1898	1902	1909	rVB	56415	100850	1.35%	0.189%
13	14.263	1926	1934	1940	rVB3	65527	148917	1.99%	0.278%
14	15.074	2068	2072	2081	rVB	49743	84699	1.13%	0.158%
15	15.521	2141	2148	2162	rBV	3165343	4863759	65.02%	9.093%
16	16.774	2355	2361	2365	rBV	2377455	3362941	44.95%	6.287%
17	16.815	2365	2368	2376	rVV	485651	717361	9.59%	1.341%
18	16.910	2380	2384	2391	rVB	133576	188766	2.52%	0.353%
19	17.198	2426	2433	2441	rBV3	39702	94801	1.27%	0.177%
20	17.657	2507	2511	2515	rVB	67992	88699	1.19%	0.166%
21	17.715	2515	2521	2528	rBV2	868090	1321695	17.67%	2.471%
22	17.845	2539	2543	2548	rBV2	109697	181885	2.43%	0.340%
23	18.586	2665	2669	2675	rBV2	51850	90634	1.21%	0.169%
24	18.727	2689	2693	2702	rVB8	49843	91952	1.23%	0.172%
25	18.851	2709	2714	2720	rBV	733797	986618	13.19%	1.845%
26	19.015	2737	2742	2749	rBV	449814	670258	8.96%	1.253%
27	19.221	2769	2777	2783	rBV	557704	967162	12.93%	1.808%
28	19.445	2809	2815	2827	rVB	5843124	7480889	100.00%	13.986%
29	19.727	2860	2863	2868	rVB	113752	141785	1.90%	0.265%
30	19.827	2877	2880	2884	rBV	108699	133524	1.78%	0.250%
31	20.715	3028	3031	3033	rBV2	142782	157485	2.11%	0.294%
32	20.750	3034	3037	3048	rVB3	391093	624152	8.34%	1.167%
33	20.956	3069	3072	3075	rBV	251686	287895	3.85%	0.538%
34	21.015	3076	3082	3086	rVV2	2210165	3282113	43.87%	6.136%
35	21.056	3086	3089	3098	rVB	262034	396409	5.30%	0.741%
36	23.709	3533	3540	3553	rVB	1157109	2756451	36.85%	5.154%

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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-BM081024.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

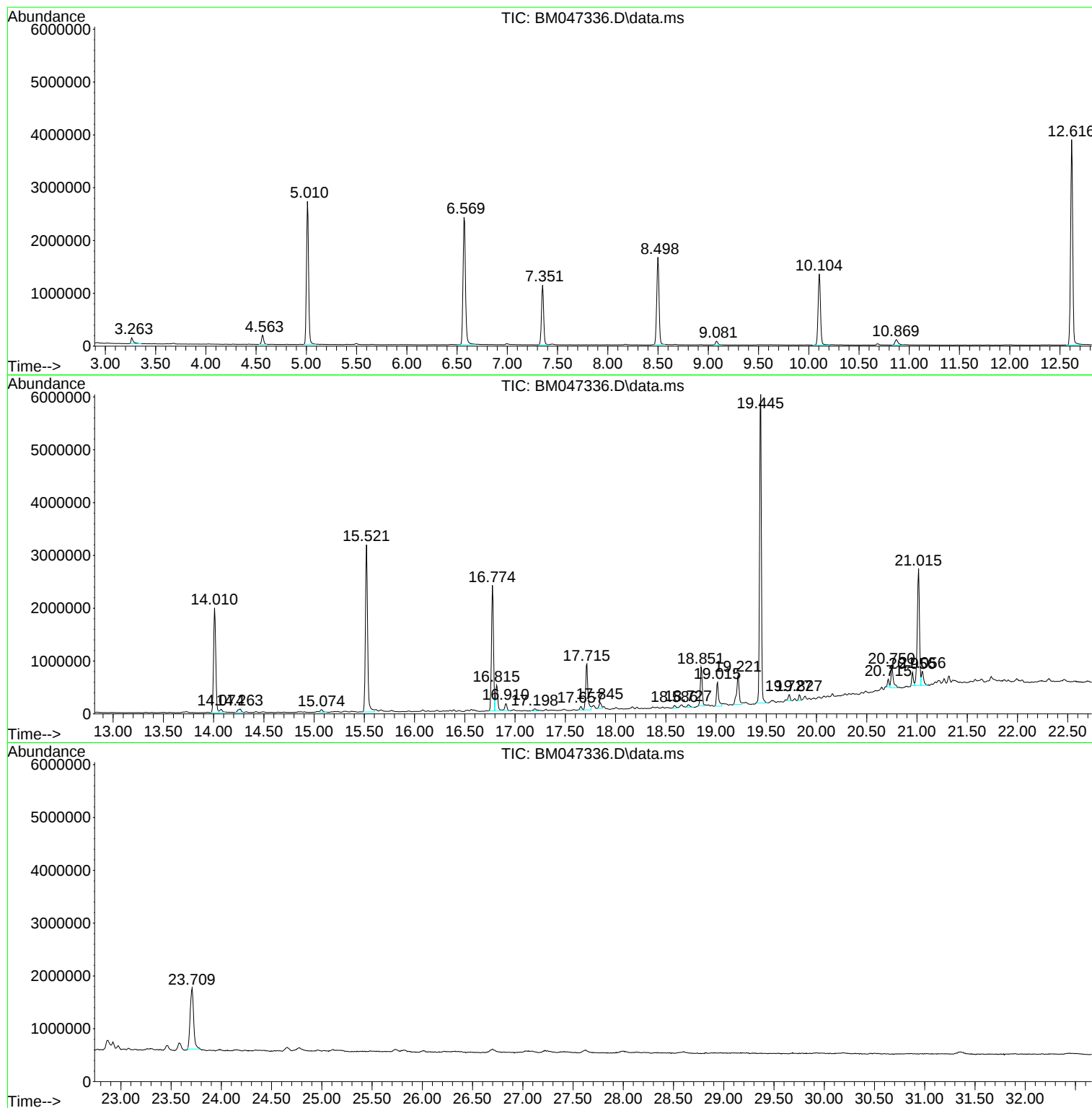
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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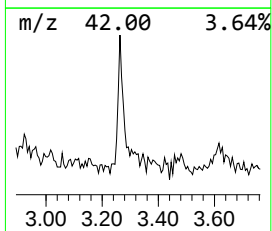
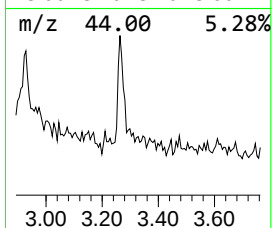
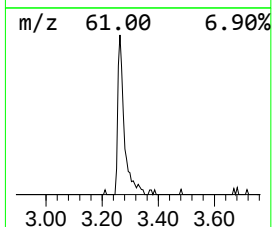
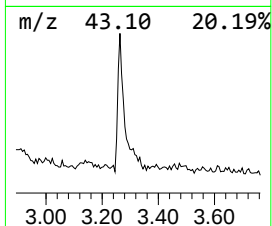
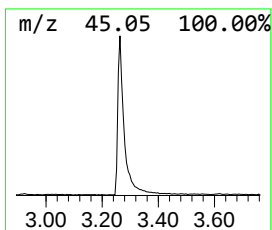
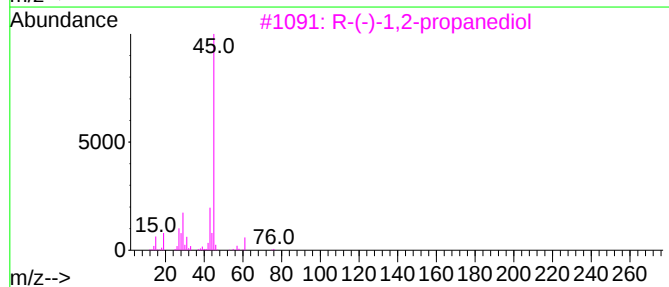
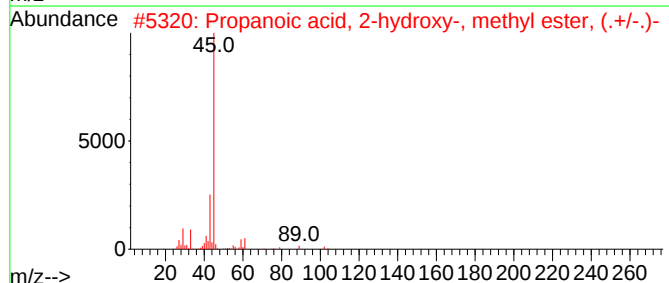
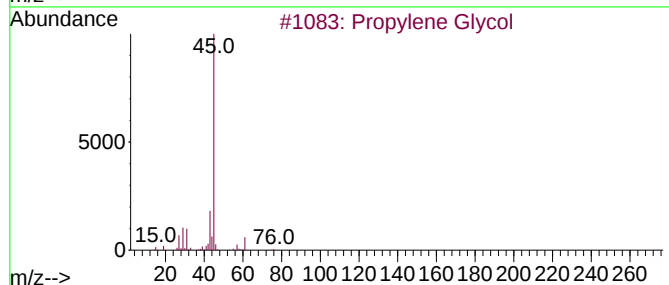
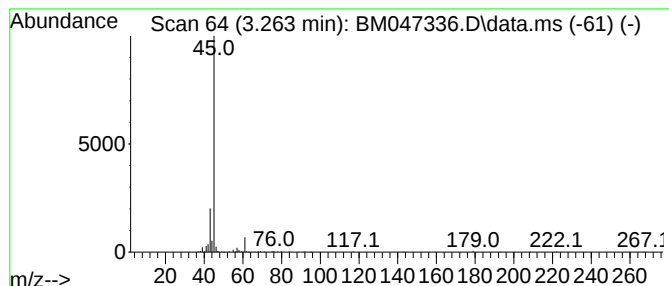
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Propylene Glycol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.263	2.07 ng	180031	1,4-Dichlorobenzene-d4	7.351

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Propylene Glycol	76	C3H8O2	000057-55-6	86
2		Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	40
3		R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	9
4		(S)-Isopropyl lactate	132	C6H12O3	063697-00-7	9
5		(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	9



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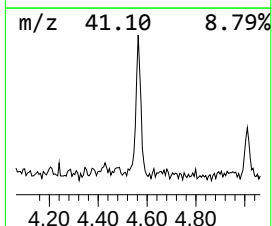
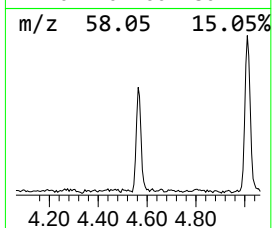
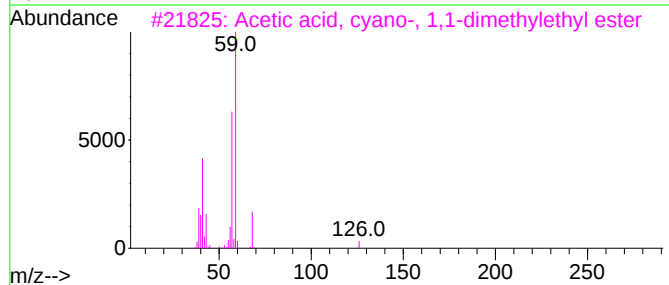
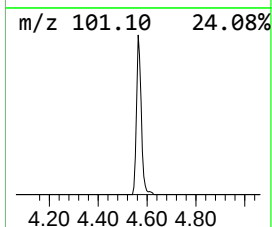
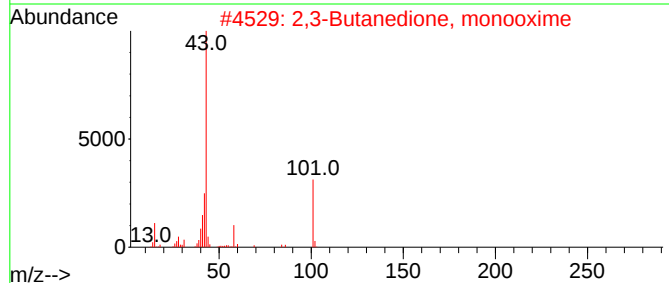
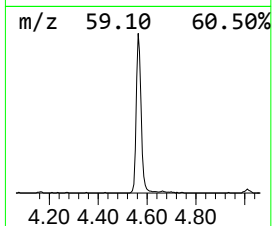
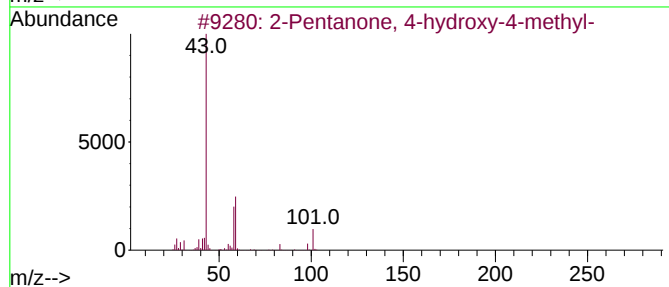
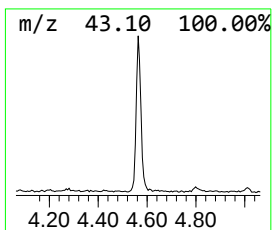
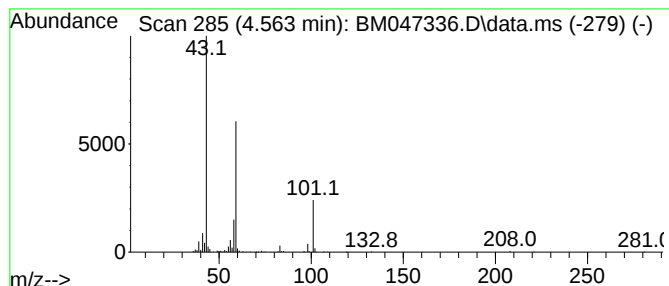
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.563	2.84 ng	247054	1,4-Dichlorobenzene-d4	7.351

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64		
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	32		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17		
4	dl-Erythro-0-methylthreonine	133	C5H11NO3	1000214-70-7	9		
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		



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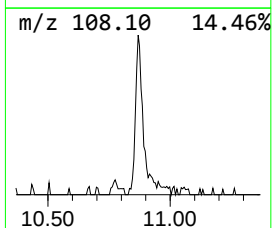
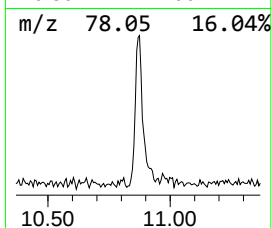
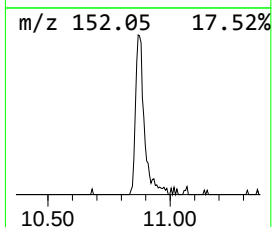
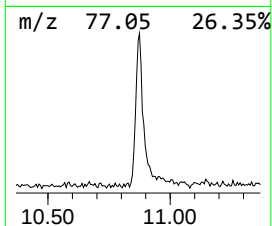
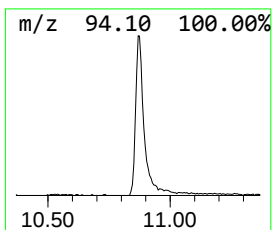
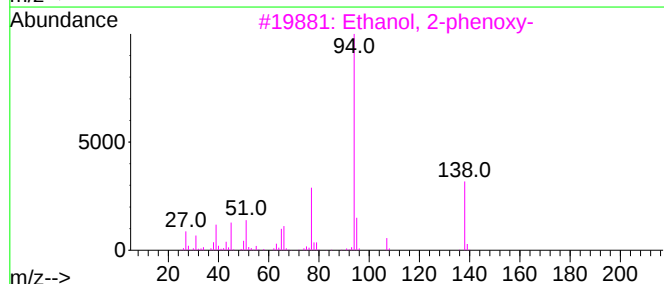
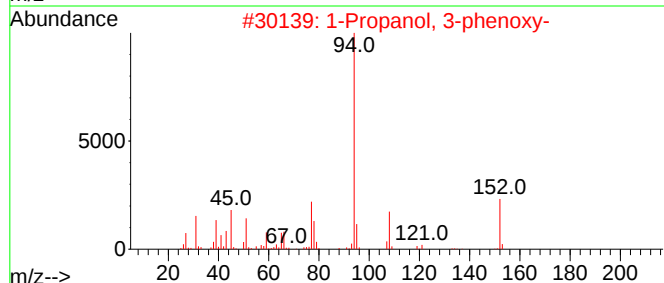
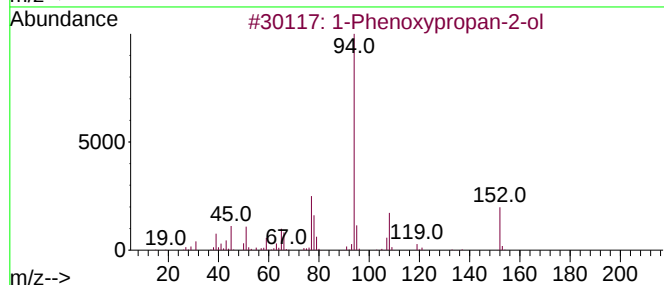
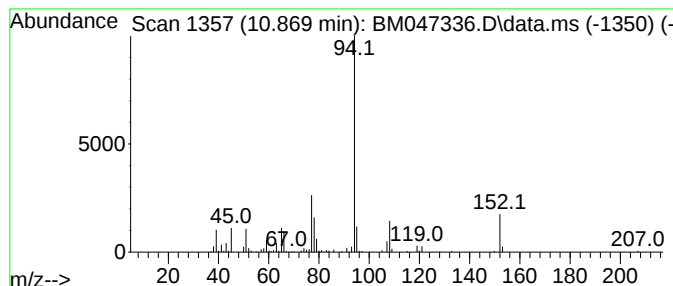
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 1-Phenoxypropan-2-ol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.869	2.07 ng	234565	Naphthalene-d8	10.104

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	96
2			1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	87
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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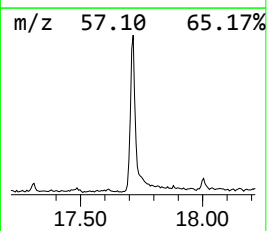
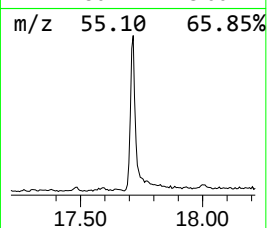
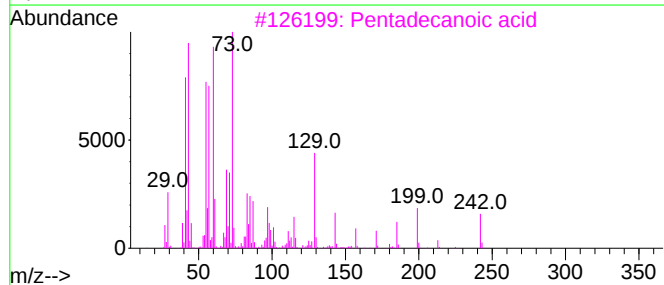
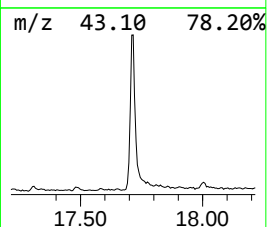
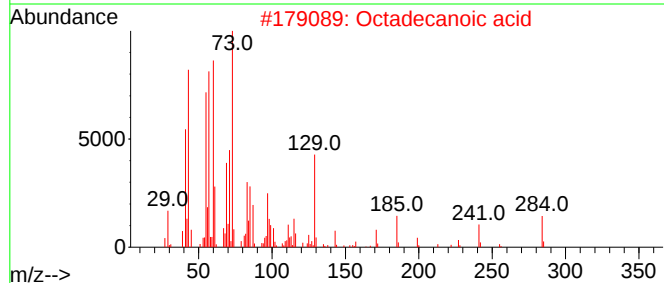
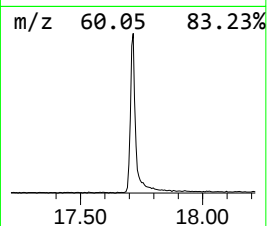
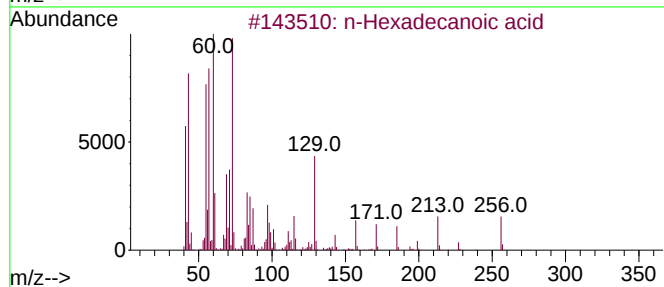
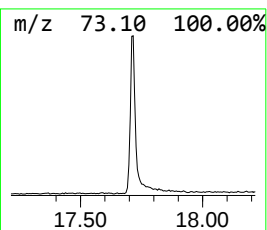
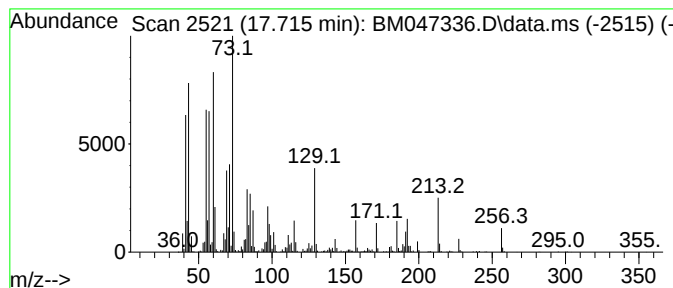
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.715	7.86 ng	1321700	Phenanthrene-d10	16.774

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	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4			Tridecanoic acid	214	C13H26O2	000638-53-9	90
5			n-Decanoic acid	172	C10H20O2	000334-48-5	76



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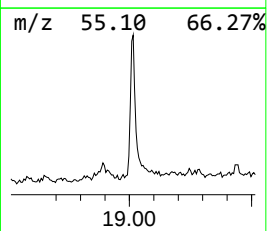
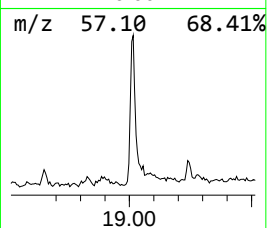
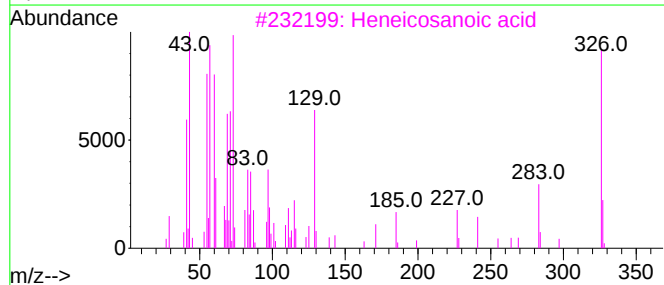
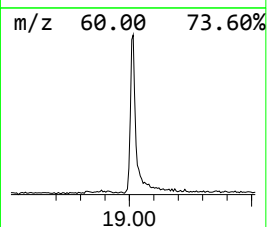
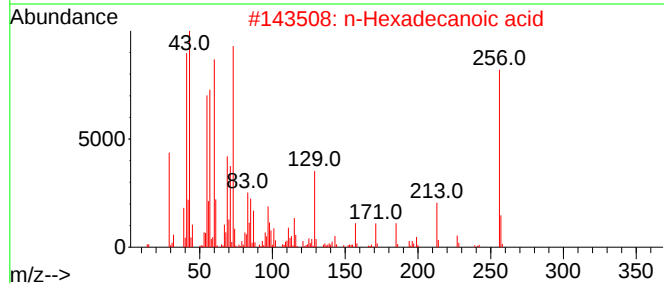
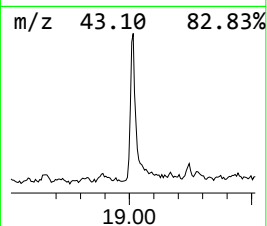
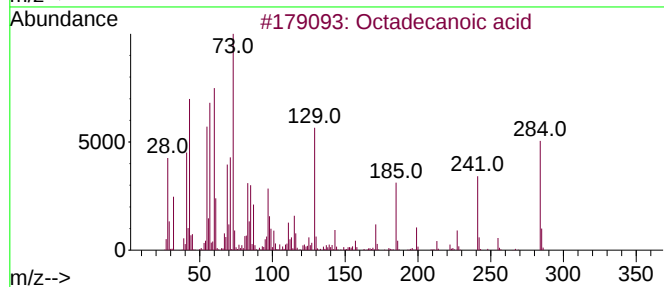
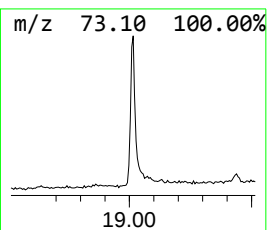
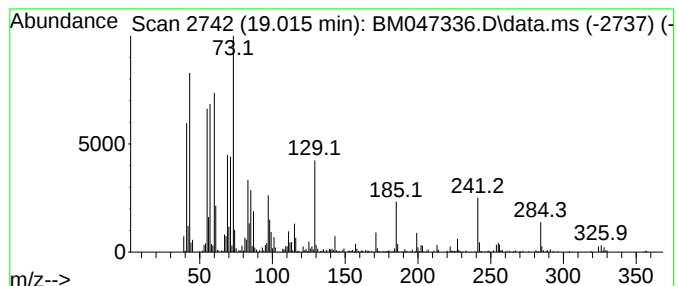
Instrument :
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.015	4.08 ng	670258	Chrysene-d12	21.015	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3	Heneicosanoic acid	326	C21H42O2	002363-71-5	93
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5	Tridecanoic acid	214	C13H26O2	000638-53-9	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082324\
Data File : BM047336.D
Acq On : 23 Aug 2024 16:48
Operator : RC/JU
Sample : P3694-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
Kingsland-Driveway

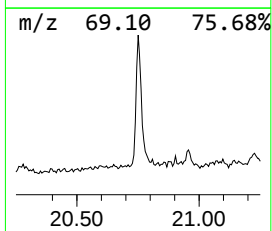
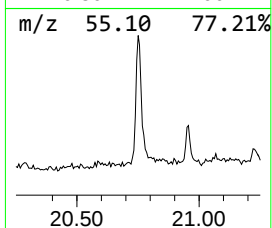
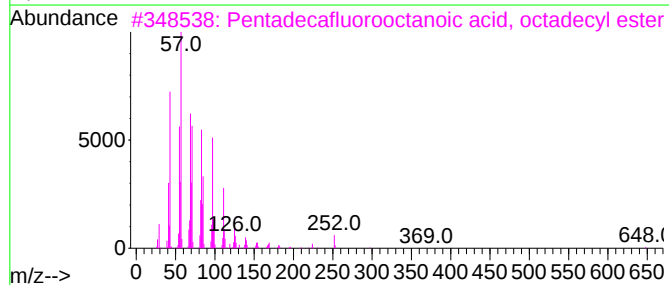
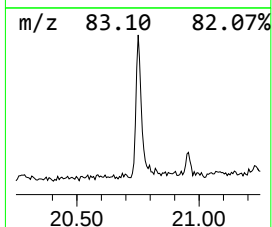
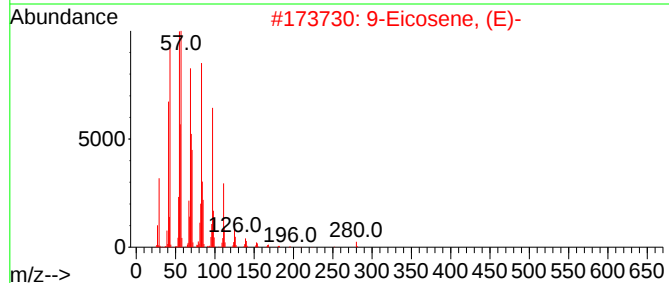
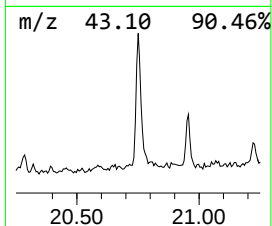
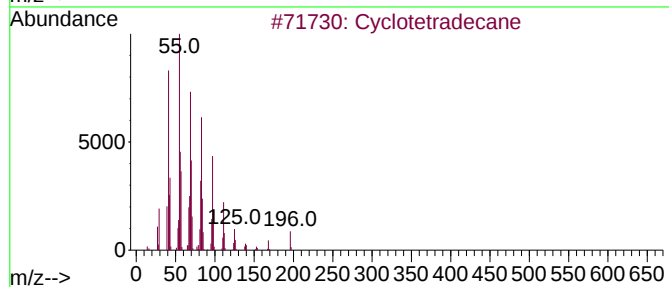
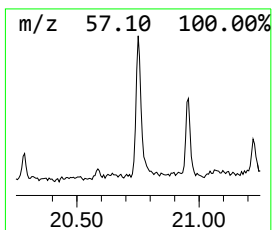
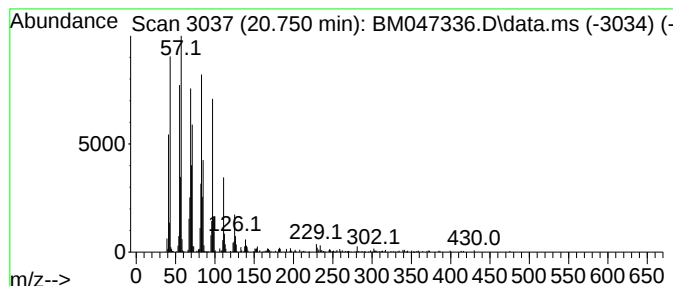
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Cyclotetradecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.750	3.80 ng	624152	Chrysene-d12	21.015

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclotetradecane	196	C14H28	000295-17-0	93
2			9-Eicosene, (E)-	280	C20H40	074685-29-3	93
3			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	93
4			Nonadecyl heptafluorobutyrate	480	C23H39F7O2	1000351-83-9	91
5			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082324\
Data File : BM047336.D
Acq On : 23 Aug 2024 16:48
Operator : RC/JU
Sample : P3694-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
Kingsland-Driveway

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.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
Propylene Glycol	3.263	2.1	ng	180031	1	7.351	1737390	20.0
2-Pentanone, 4-...	4.563	2.8	ng	247054	1	7.351	1737390	20.0
1-Phenoxypropan...	10.869	2.1	ng	234565	2	10.104	2271290	20.0
n-Hexadecanoic ...	17.715	7.9	ng	1321700	4	16.774	3362940	20.0
Octadecanoic acid	19.015	4.1	ng	670258	5	21.015	3282110	20.0
Cyclotetradecane	20.750	3.8	ng	624152	5	21.015	3282110	20.0