

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082024\
 Data File : BM047286.D
 Acq On : 21 Aug 2024 01:33
 Operator : RC/JU
 Sample : P3643-05
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 917-J-SD-0-0.5-081524

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: BM047286.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.569	278	286	294	rBV	180041	258619	5.34%	0.601%
2	5.016	355	362	378	rBV	2813671	4060385	83.80%	9.439%
3	6.569	619	626	638	rBV	2567774	4155347	85.76%	9.659%
4	6.675	640	644	651	rVB2	63242	108068	2.23%	0.251%
5	7.357	752	760	769	rBV	1057036	1647684	34.00%	3.830%
6	8.504	948	955	968	rBV	1712038	2699697	55.72%	6.276%
7	9.087	1048	1054	1066	rBV	74507	136239	2.81%	0.317%
8	10.110	1221	1228	1240	rBV	1294062	2135131	44.06%	4.963%
9	10.692	1322	1327	1337	rBV4	29531	54517	1.13%	0.127%
10	10.875	1352	1358	1371	rBV	154410	320571	6.62%	0.745%
11	12.622	1648	1655	1667	rBV	3202833	4845461	100.00%	11.264%
12	13.910	1864	1874	1878	rBV6	27007	68745	1.42%	0.160%
13	14.016	1886	1892	1902	rBV	1827418	2668235	55.07%	6.202%
14	14.251	1926	1932	1933	rBV4	49110	61448	1.27%	0.143%
15	14.269	1933	1935	1942	rVB2	54529	74817	1.54%	0.174%
16	15.527	2142	2149	2168	rBV	2667707	4173730	86.14%	9.702%
17	16.780	2356	2362	2367	rBV	2020513	2857724	58.98%	6.643%
18	16.821	2367	2369	2373	rVB	101797	116214	2.40%	0.270%
19	16.915	2381	2385	2392	rVB4	40826	69329	1.43%	0.161%
20	17.715	2516	2521	2534	rBV	343754	587038	12.12%	1.365%
21	18.857	2710	2715	2723	rBV	319547	476480	9.83%	1.108%
22	19.015	2738	2742	2750	rBV2	191062	285435	5.89%	0.664%
23	19.221	2770	2777	2785	rBV	226272	368056	7.60%	0.856%
24	19.445	2810	2815	2826	rBV	3593909	4472624	92.31%	10.397%
25	20.756	3034	3038	3043	rBV	254404	344380	7.11%	0.801%
26	20.868	3053	3057	3060	rBV	130224	159800	3.30%	0.371%
27	20.927	3064	3067	3071	rVB	106133	116606	2.41%	0.271%
28	21.015	3077	3082	3087	rBV	1878050	2579524	53.24%	5.996%
29	22.980	3413	3416	3422	rVB	213206	353225	7.29%	0.821%
30	23.709	3533	3540	3557	rVB	1165429	2763935	57.04%	6.425%

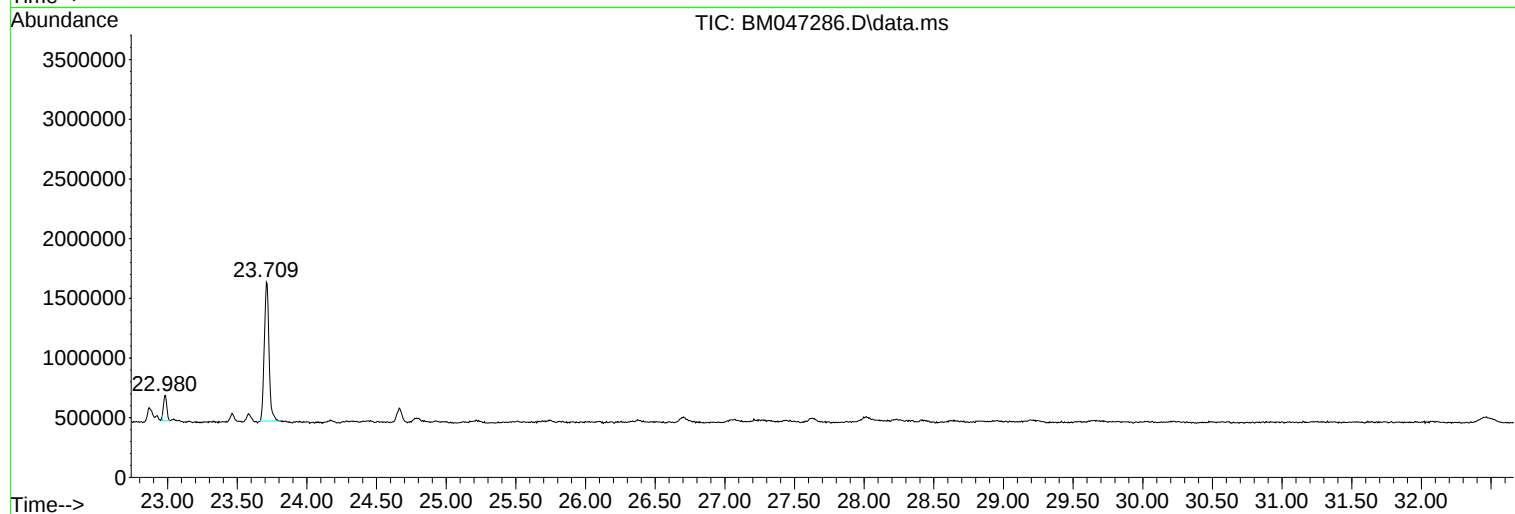
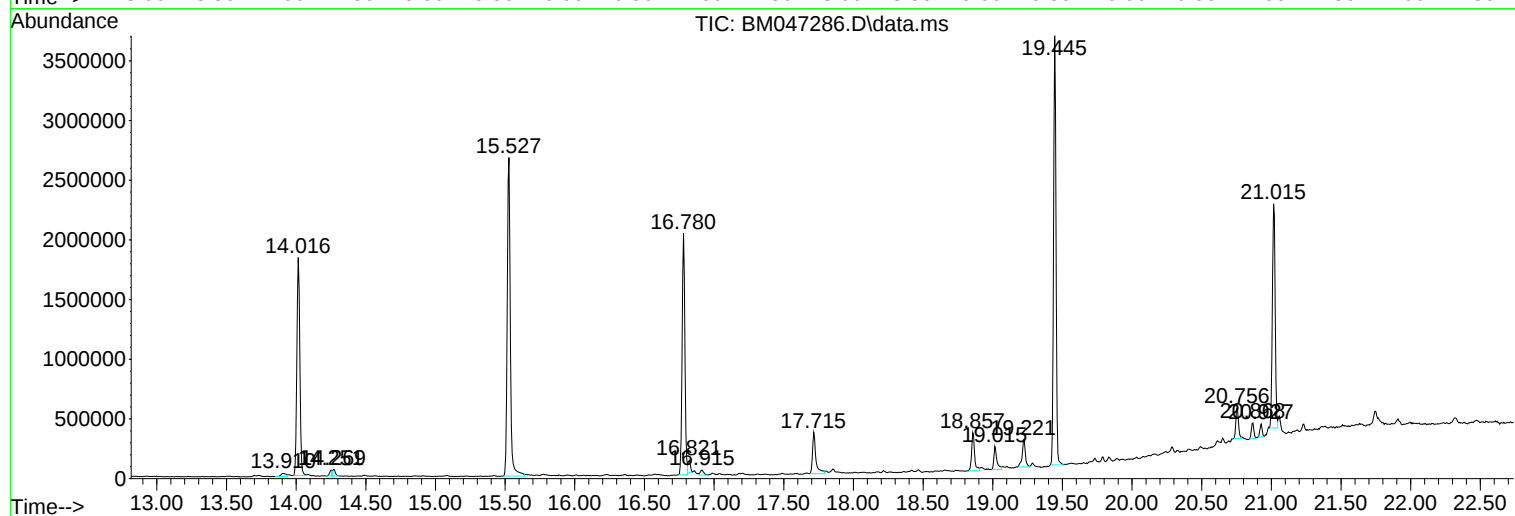
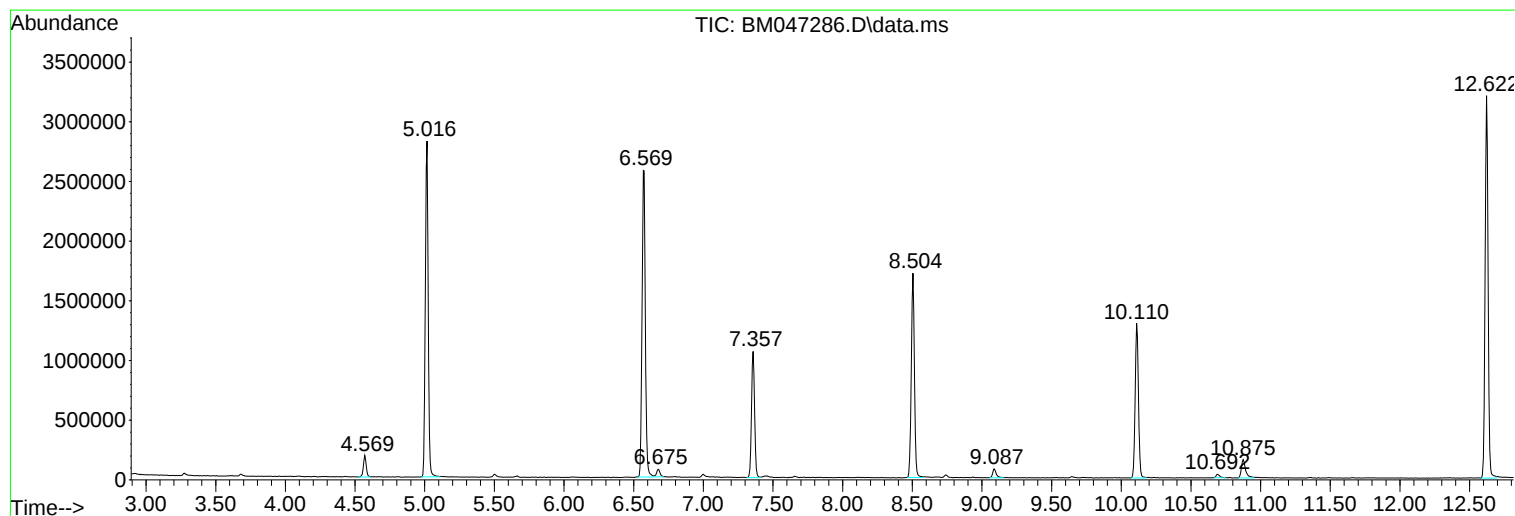
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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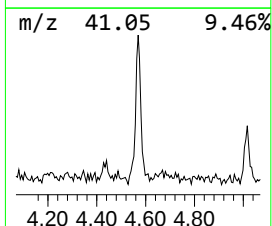
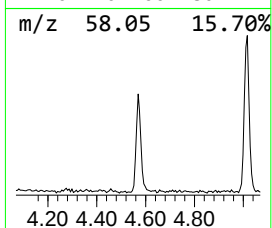
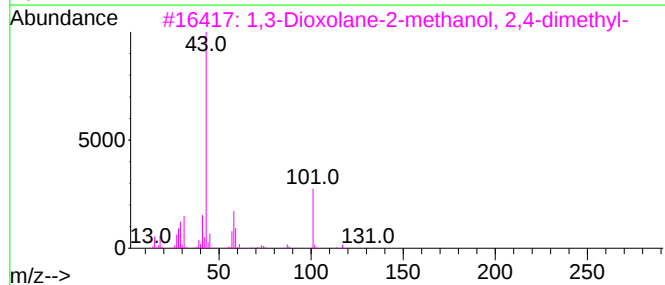
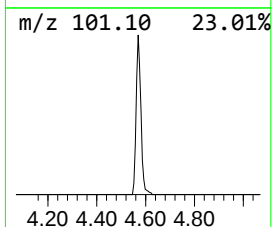
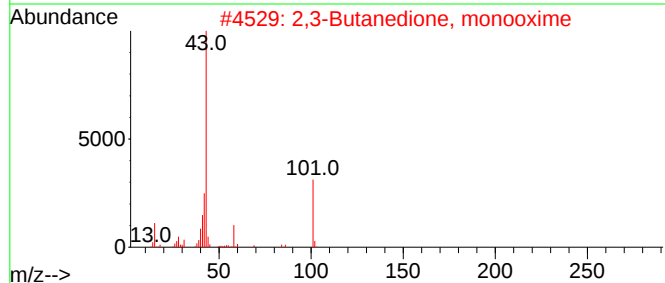
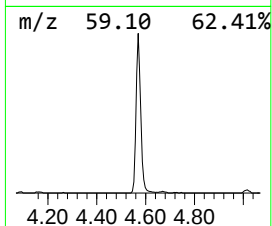
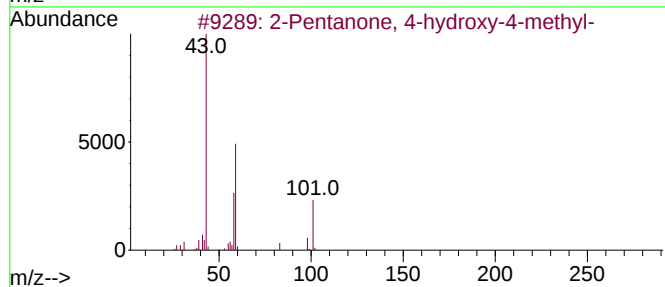
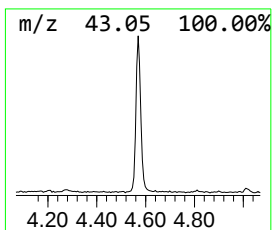
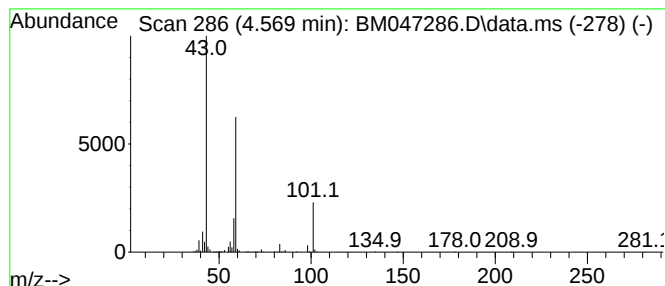
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.569	3.14 ng	258619	1,4-Dichlorobenzene-d4	7.357

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	47	
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35	
3	1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	25	
4	Tetraglyme	222	C10H22O5	000143-24-8	25	
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9	



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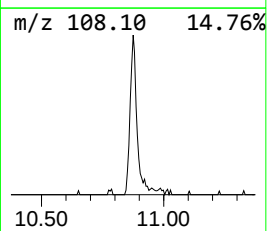
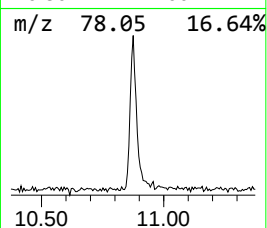
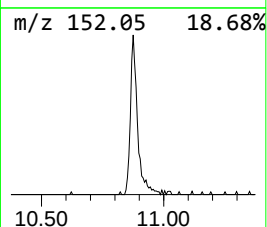
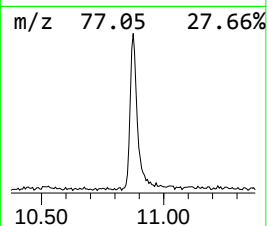
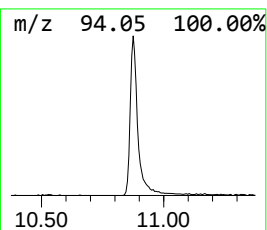
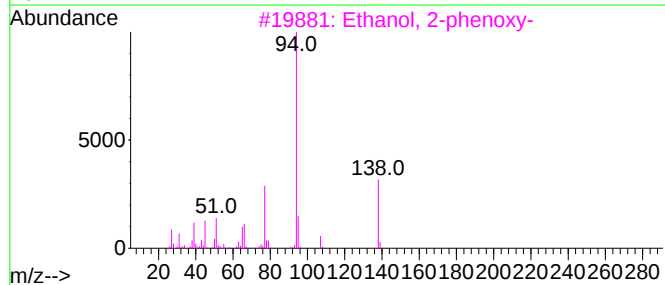
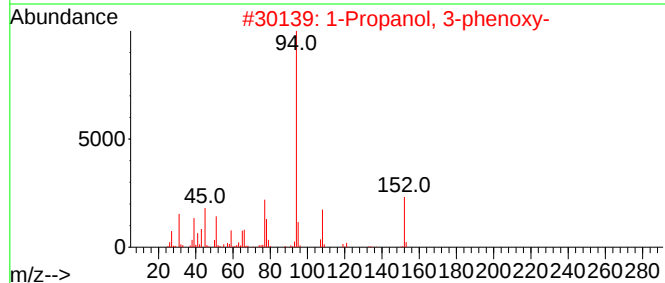
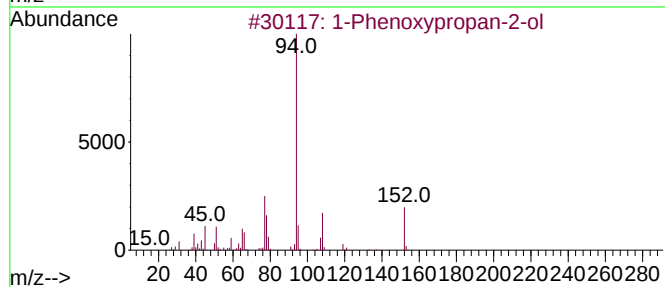
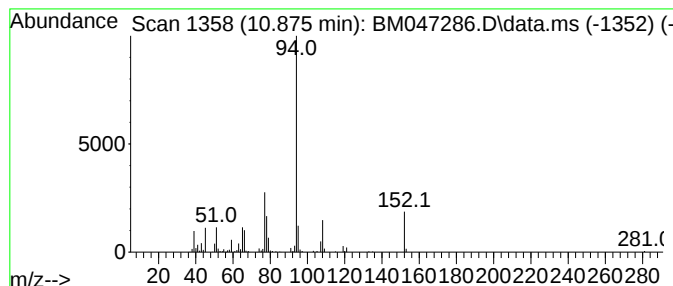
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Peak Number 2 1-Phenoxypropan-2-ol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.875	3.00 ng	320571	Naphthalene-d8	10.110

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	83
3		Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
4		1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	64
5		3-(.alpha.-Hydroxyethyl)-aniline	137	C8H11NO	002454-37-7	59



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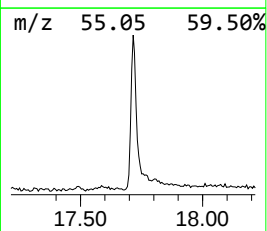
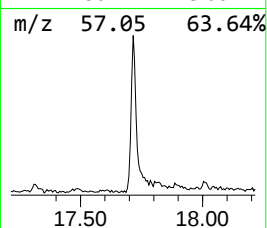
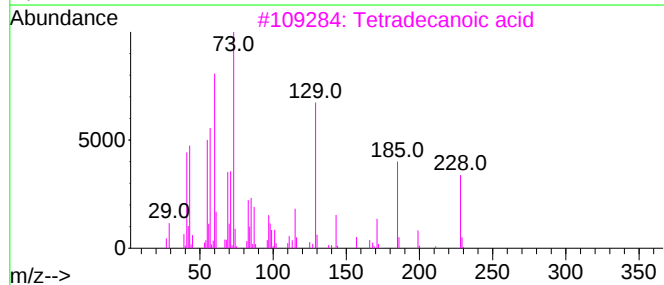
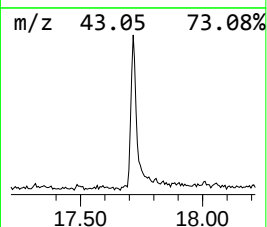
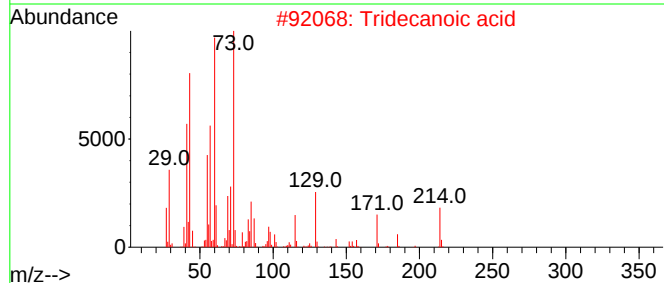
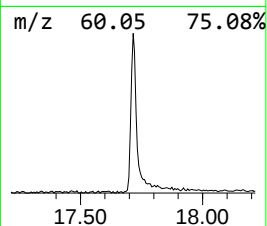
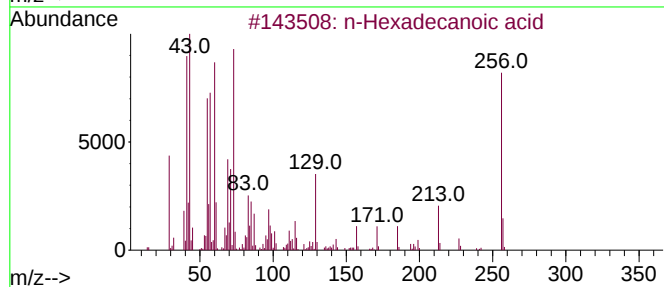
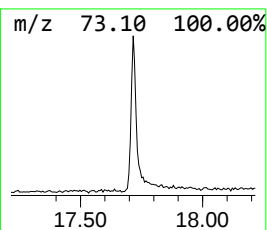
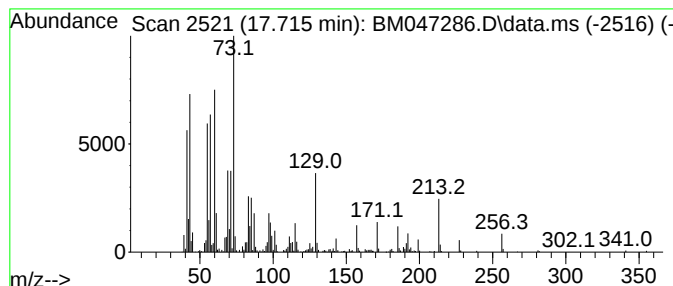
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.715	4.11 ng	587038	Phenanthrene-d10	16.780

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	89
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
5			Octadecanoic acid	284	C18H36O2	000057-11-4	70



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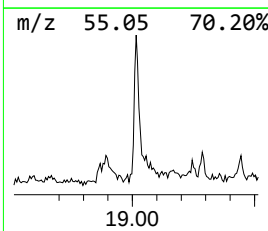
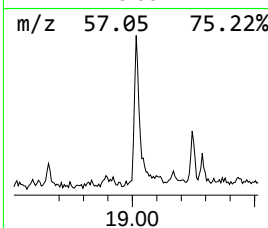
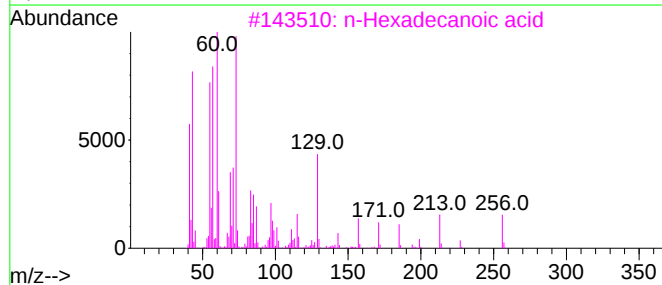
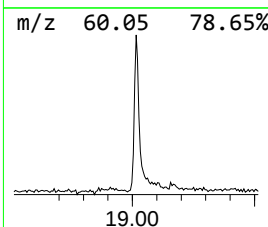
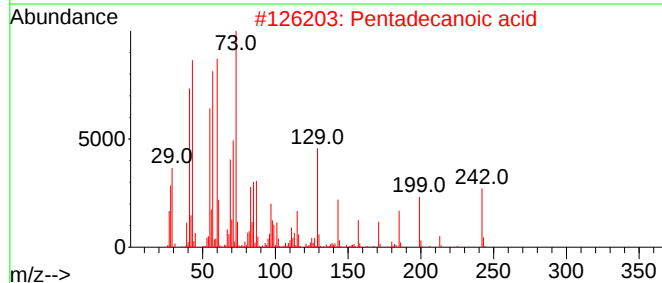
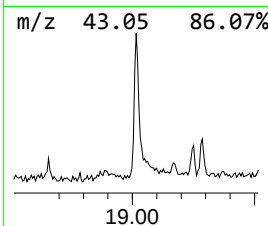
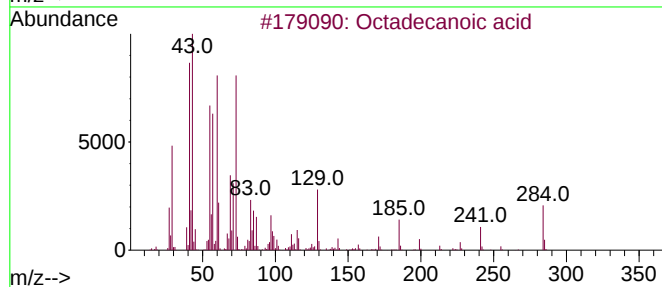
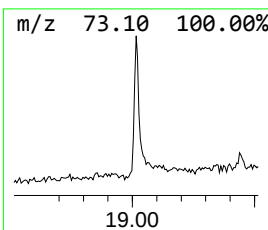
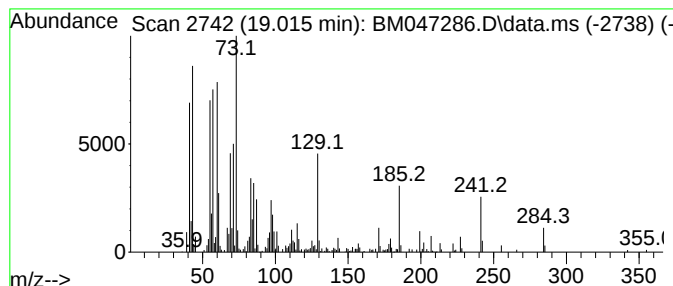
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Peak Number 4 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.015	2.21 ng	285435	Chrysene-d12	21.015

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	98
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	68
4			Tridecanoic acid	214	C13H26O2	000638-53-9	62
5			n-Decanoic acid	172	C10H20O2	000334-48-5	62



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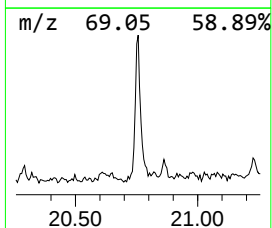
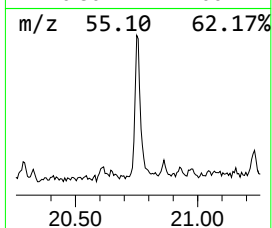
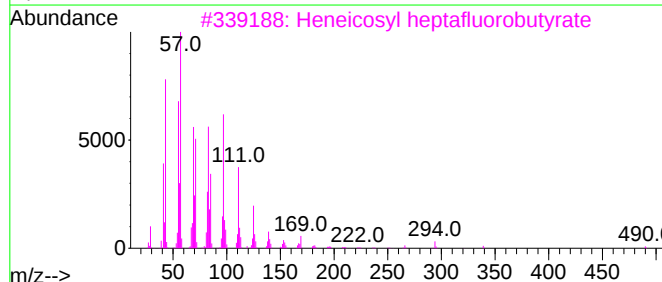
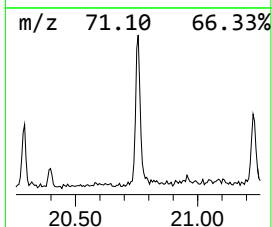
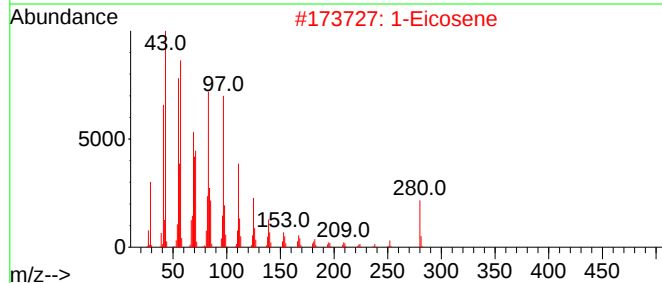
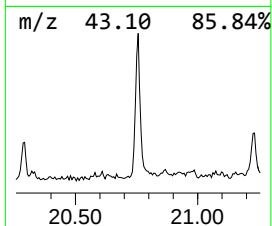
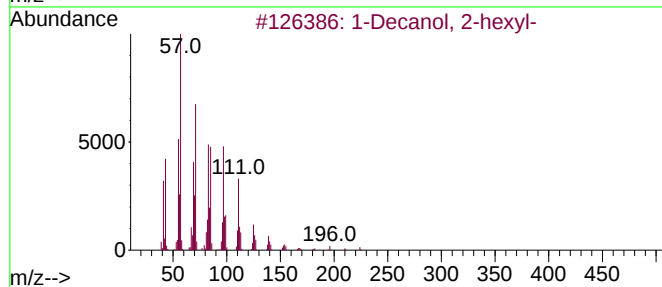
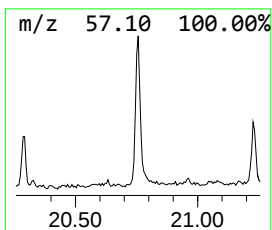
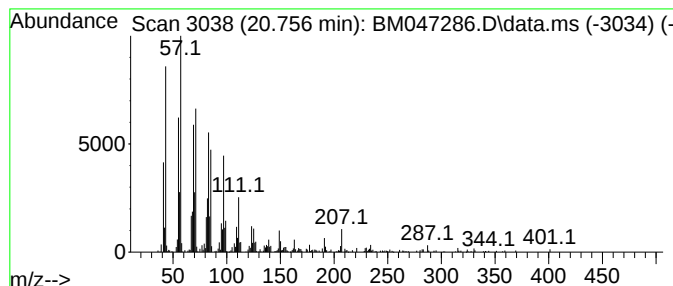
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Peak Number 5 1-Decanol, 2-hexyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.756	2.67 ng	344380	Chrysene-d12	21.015

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Decanol, 2-hexyl-			242	C16H34O	002425-77-6	83
2	1-Eicosene			280	C20H40	003452-07-1	78
3	Heneicosyl heptafluorobutyrate			508	C25H43F7O2	1000351-83-8	76
4	Ethanol, 2-(tetradecyloxy)-			258	C16H34O2	002136-70-1	76
5	Pentadecafluorooctanoic acid, oc...			666	C26H37F15O2	1000406-04-8	76



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917-J-SD-0-0.5-081524

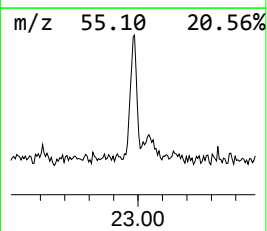
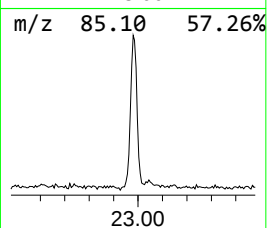
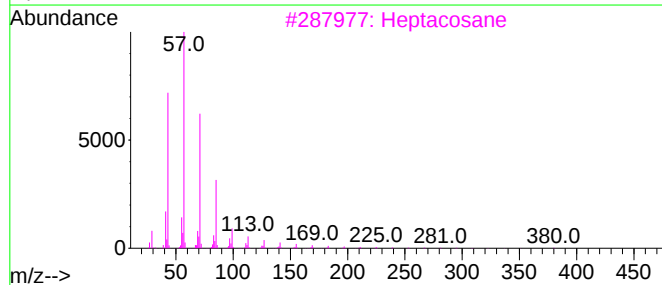
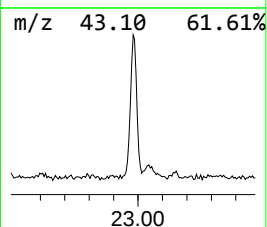
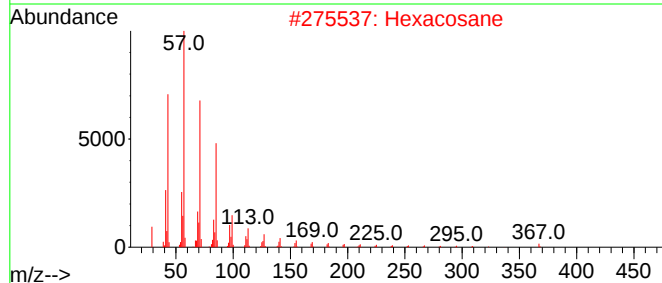
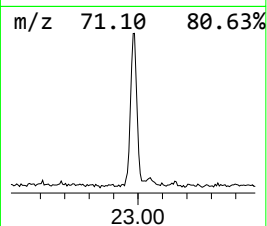
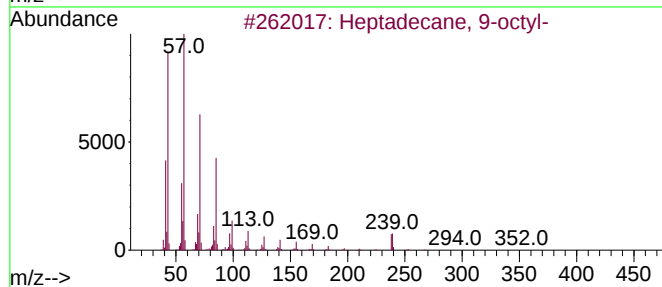
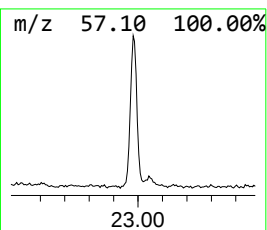
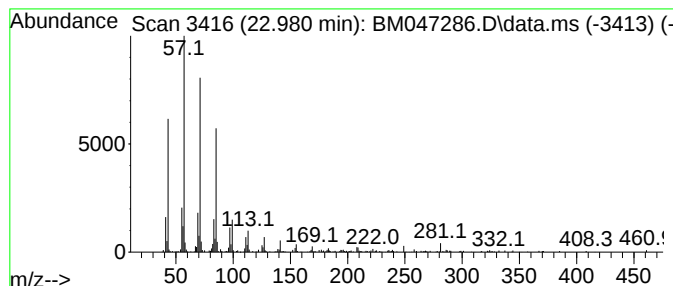
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Heptadecane, 9-octyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.980	2.56 ng	353225	Perylene-d12	23.709

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	93
2		Hexacosane	366	C26H54	000630-01-3	87
3		Heptacosane	380	C27H56	000593-49-7	87
4		Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	87
5		Tricosane	324	C23H48	000638-67-5	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082024\
Data File : BM047286.D
Acq On : 21 Aug 2024 01:33
Operator : RC/JU
Sample : P3643-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
917-J-SD-0-0.5-081524

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.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-Pentanone, 4-...	4.569	3.1	ng	258619	1	7.357	1647680	20.0
1-Phenoxypropan...	10.875	3.0	ng	320571	2	10.110	2135130	20.0
n-Hexadecanoic ...	17.715	4.1	ng	587038	4	16.780	2857720	20.0
Octadecanoic acid	19.015	2.2	ng	285435	5	21.015	2579520	20.0
1-Decanol, 2-he...	20.756	2.7	ng	344380	5	21.015	2579520	20.0
Heptadecane, 9-...	22.980	2.6	ng	353225	6	23.709	2763940	20.0