

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082324\
 Data File : BM047339.D
 Acq On : 23 Aug 2024 18:47
 Operator : RC/JU
 Sample : P3640-01
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 SP-1-COMP

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: BM047339.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.257	60	63	77	rBV	260667	390744	3.55%	0.575%
2	4.563	278	285	292	rBV	266161	370673	3.37%	0.545%
3	5.010	355	361	379	rBV	3721887	5470583	49.73%	8.049%
4	6.575	620	627	641	rBV	3494115	5709046	51.90%	8.400%
5	6.987	692	697	707	rBV	78530	152069	1.38%	0.224%
6	7.351	752	759	768	rBV	1311703	1993715	18.12%	2.933%
7	8.498	945	954	967	rBV	2377599	3887530	35.34%	5.720%
8	10.104	1219	1227	1245	rBV	1585750	2622317	23.84%	3.858%
9	10.869	1350	1357	1371	rBV	261106	545696	4.96%	0.803%
10	12.616	1645	1654	1671	rBV	5756741	8881100	80.73%	13.067%
11	14.010	1884	1891	1901	rBV	2364951	3506877	31.88%	5.160%
12	14.245	1925	1931	1932	rBV	113473	127129	1.16%	0.187%
13	14.263	1932	1934	1940	rVB	134171	182512	1.66%	0.269%
14	14.845	2028	2033	2040	rBV	90616	124114	1.13%	0.183%
15	15.521	2141	2148	2159	rBV	4112749	6076686	55.24%	8.941%
16	16.774	2356	2361	2366	rBV	2658454	3856029	35.05%	5.674%
17	16.815	2366	2368	2373	rVB	202908	241219	2.19%	0.355%
18	16.904	2379	2383	2392	rVB2	89242	152835	1.39%	0.225%
19	17.651	2506	2510	2515	rBV2	123738	180954	1.64%	0.266%
20	17.715	2515	2521	2529	rBV2	831329	1235441	11.23%	1.818%
21	18.856	2709	2715	2719	rBV	554103	782914	7.12%	1.152%
22	19.009	2738	2741	2750	rBV	206190	301115	2.74%	0.443%
23	19.221	2770	2777	2783	rBV	406046	641784	5.83%	0.944%
24	19.445	2809	2815	2826	rVB	8953778	11000641	100.00%	16.186%
25	20.750	3033	3037	3047	rVB2	956868	1436280	13.06%	2.113%
26	20.956	3068	3072	3075	rBV	706795	795280	7.23%	1.170%
27	21.015	3076	3082	3086	rBV	2383798	3305116	30.04%	4.863%
28	21.762	3206	3209	3221	rVB	486494	851355	7.74%	1.253%
29	23.709	3533	3540	3554	rVB	1327527	3143375	28.57%	4.625%

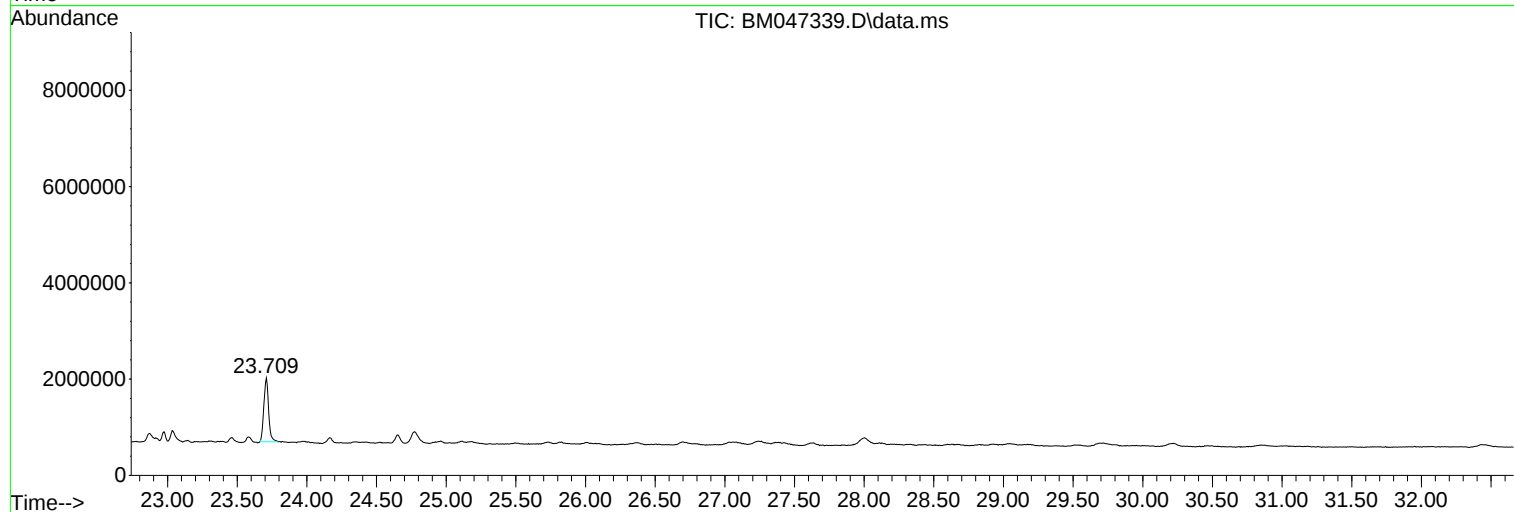
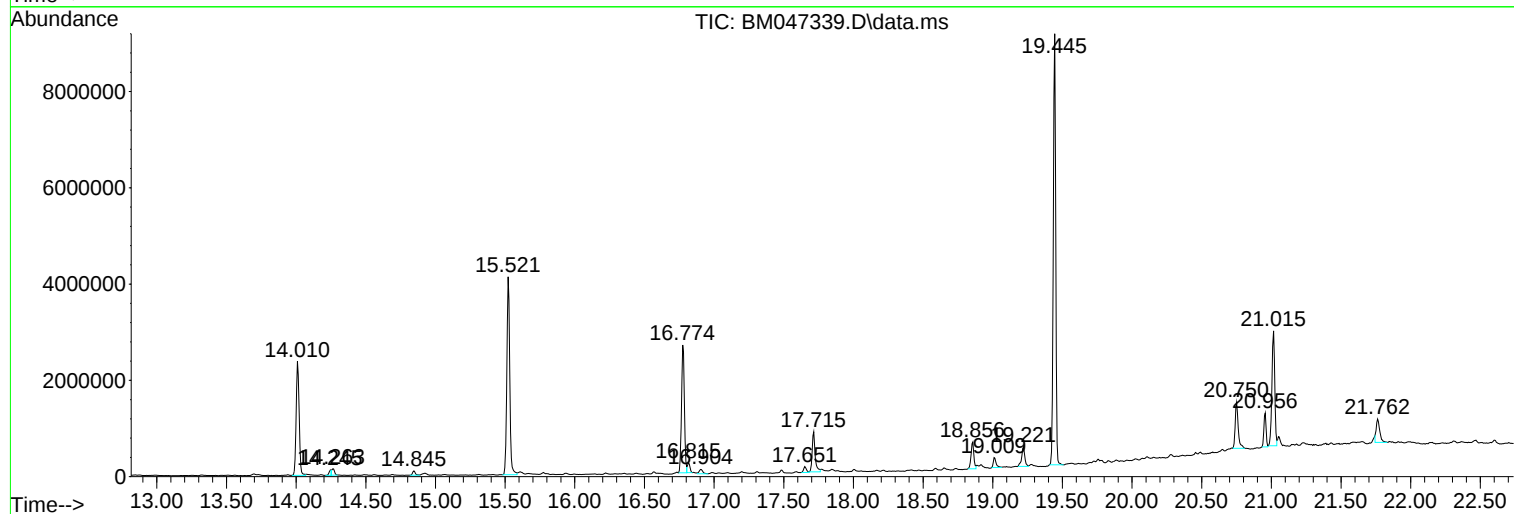
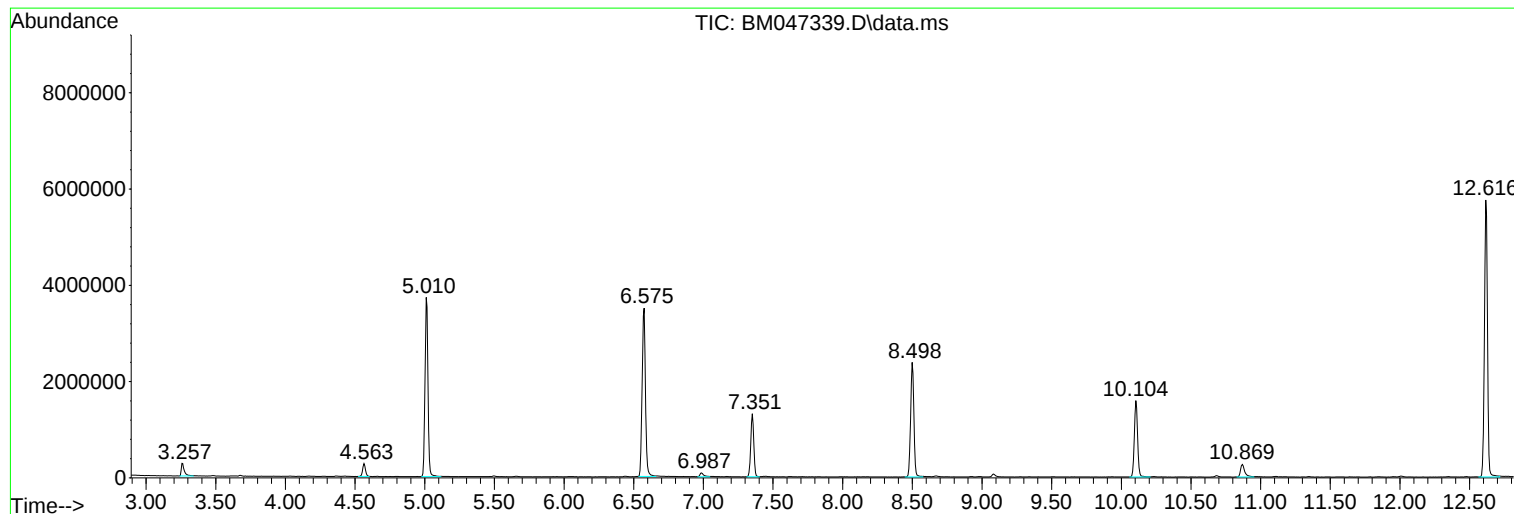
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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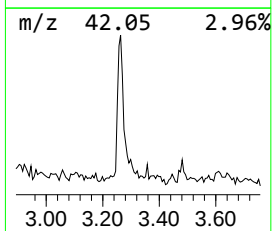
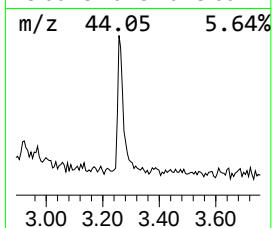
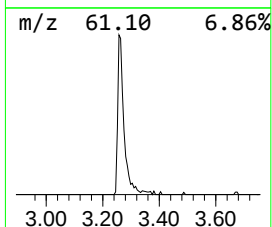
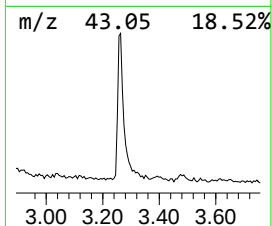
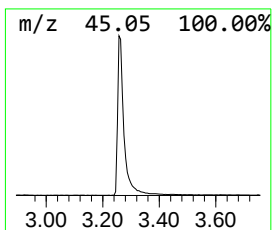
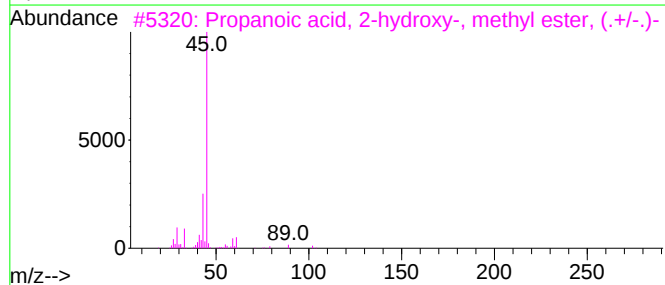
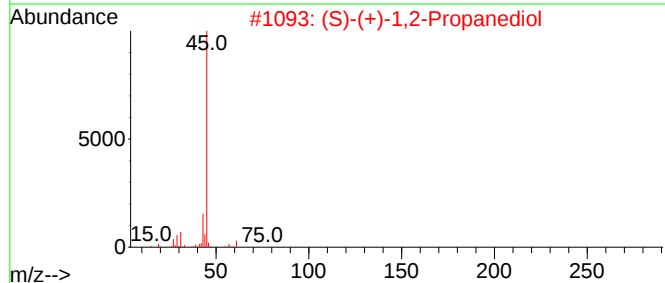
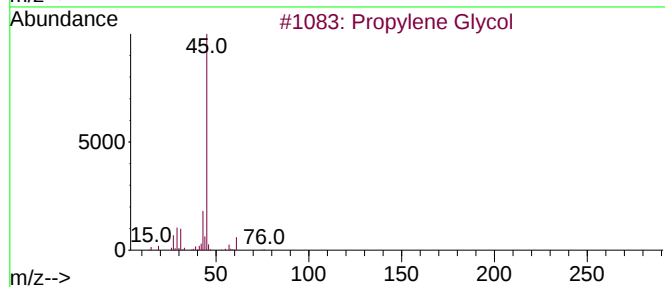
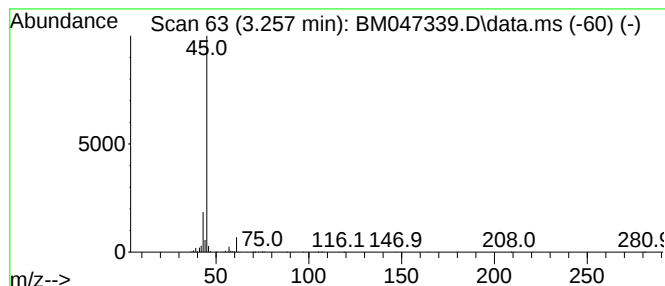
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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Peak Number 1 Propylene Glycol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.257	3.92 ng	390744	1,4-Dichlorobenzene-d4	7.351

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propylene Glycol	76	C3H8O2	000057-55-6	90
2			(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	43
3			Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	40
4			Isopropyl Alcohol	60	C3H8O	000067-63-0	9
5			Propane, 2-ethoxy-	88	C5H12O	000625-54-7	9



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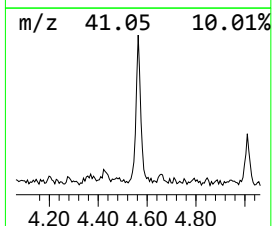
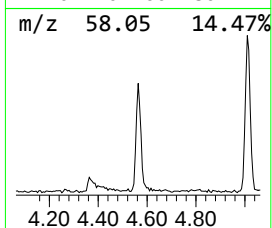
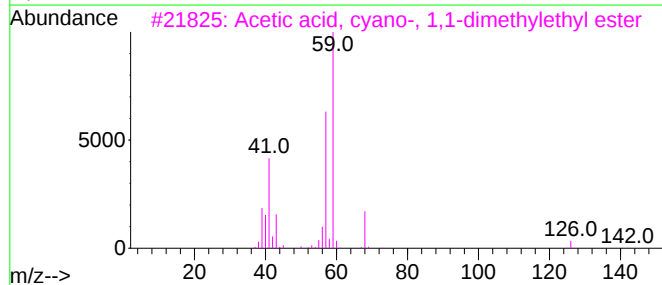
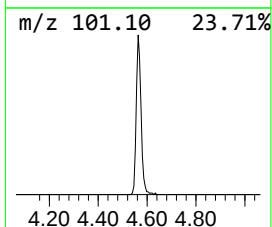
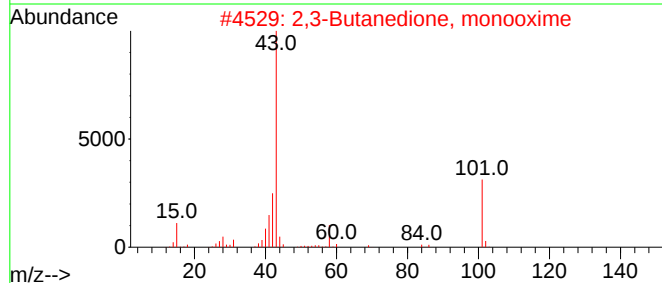
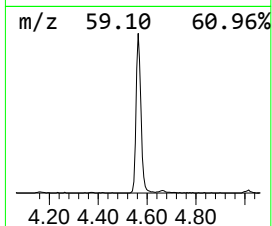
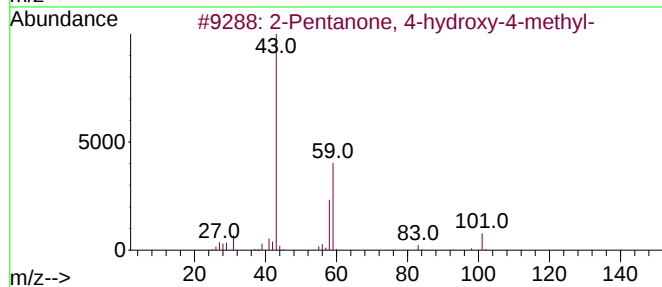
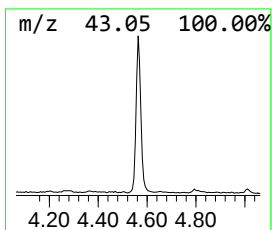
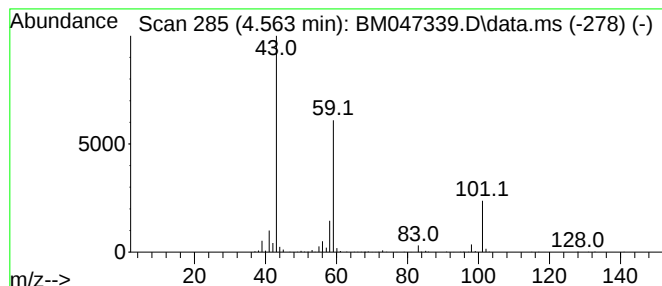
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.563	3.72 ng	370673	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	72
2			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4			Hexanamide	115	C6H13NO	000628-02-4	9
5			dl-Erythro-0-methylthreonine	133	C5H11NO3	1000214-70-7	9



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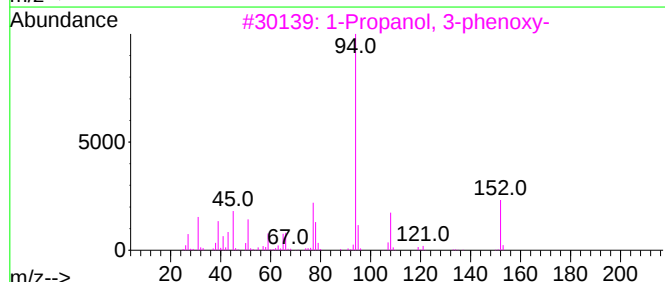
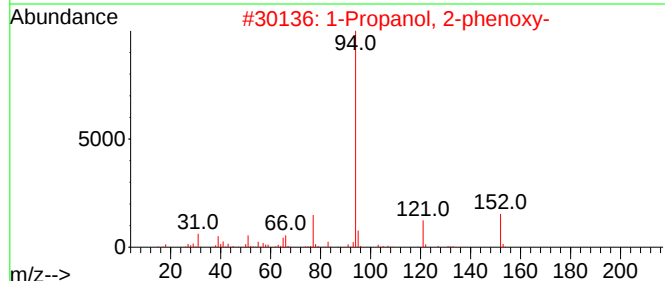
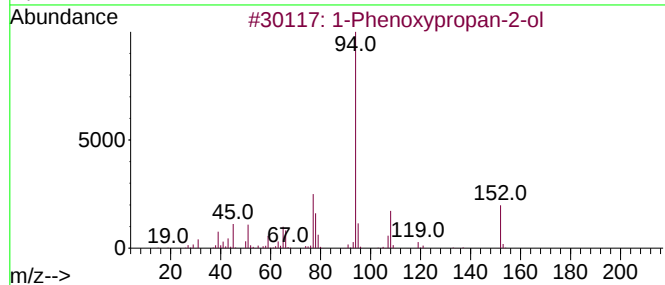
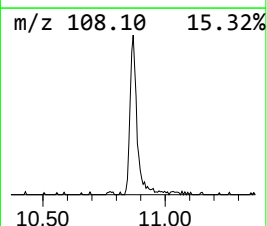
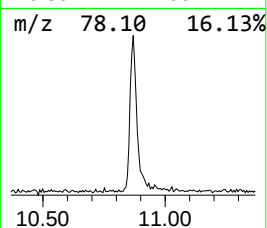
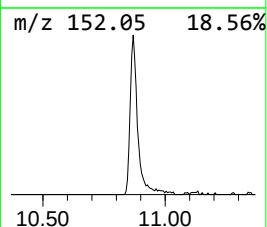
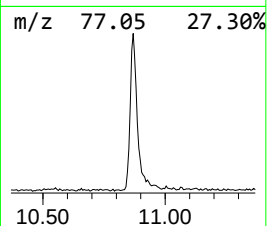
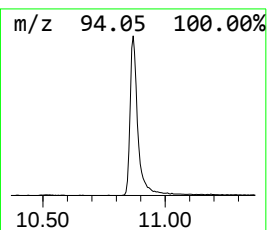
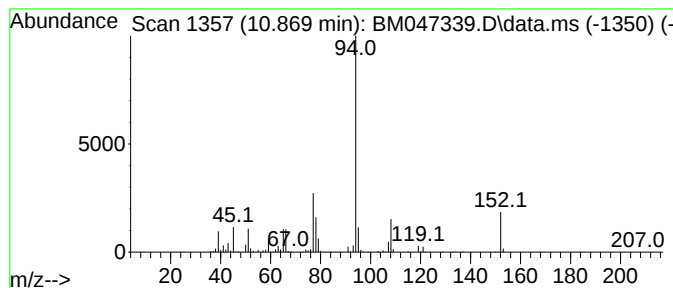
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 1-Phenoxypropan-2-ol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.869	4.16 ng	545696	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, 2-phenoxy-	152	C9H12O2	004169-04-4	64
3			1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	64
4			Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
5			Carbonic acid, (3,4,4-trimethyl-...	252	C13H16O5	109123-69-5	59



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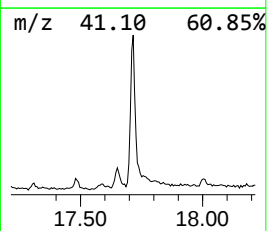
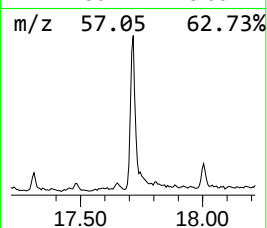
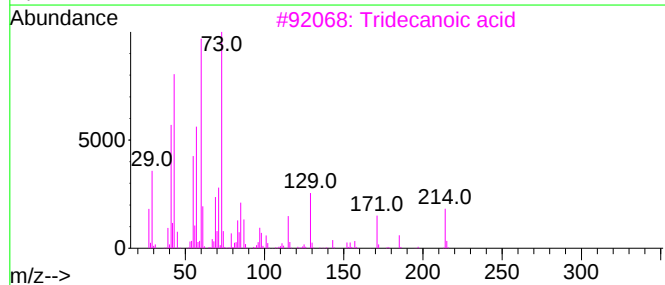
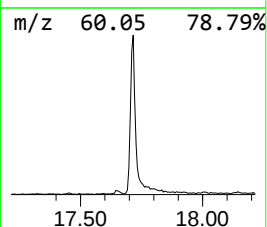
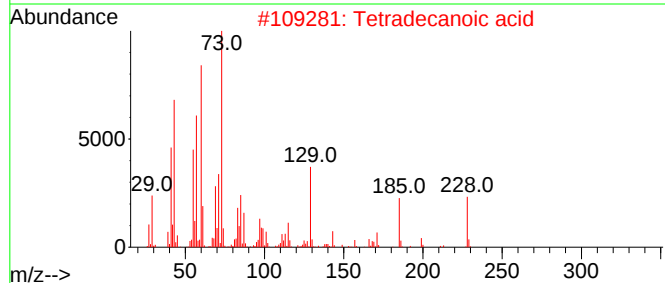
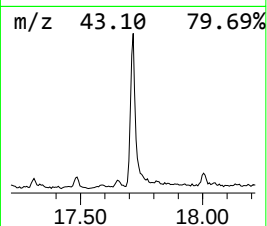
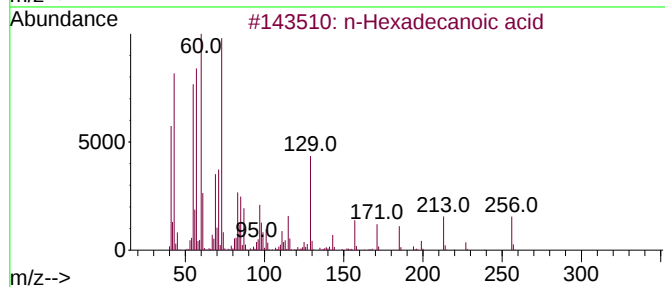
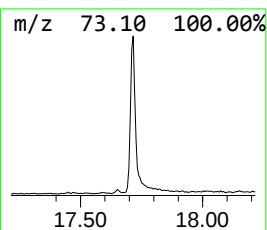
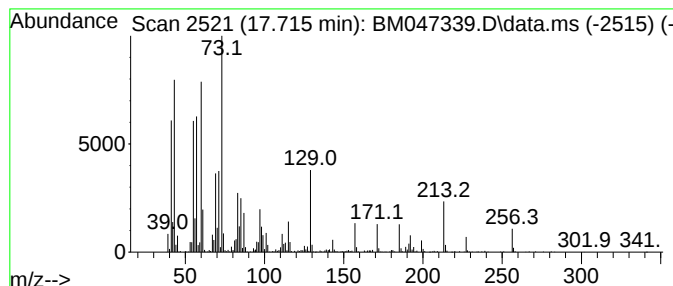
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.715	6.41 ng	1235440	Phenanthrene-d10	16.774

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3			Tridecanoic acid	214	C13H26O2	000638-53-9	89
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5			Dodecanoic acid	200	C12H24O2	000143-07-7	64



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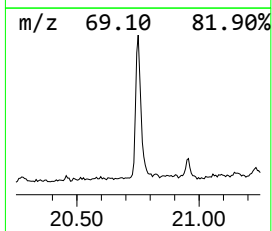
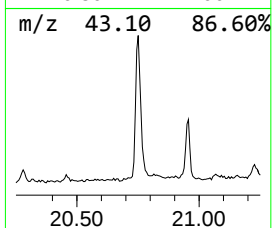
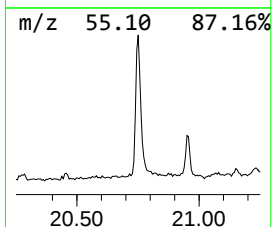
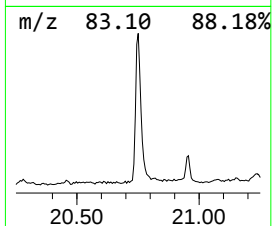
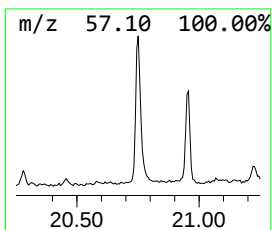
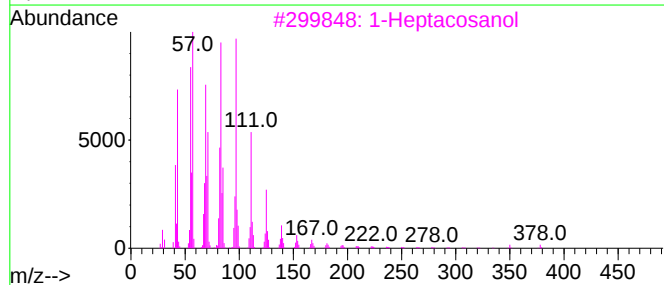
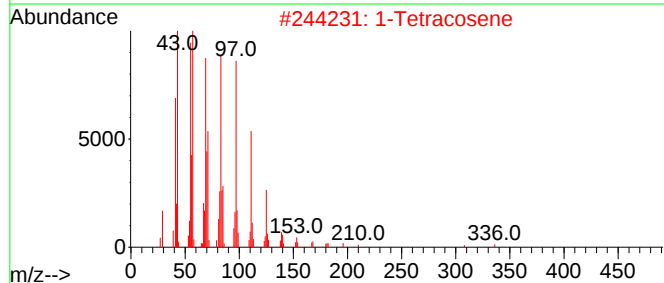
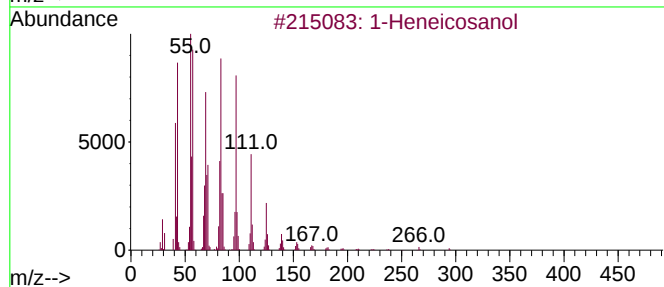
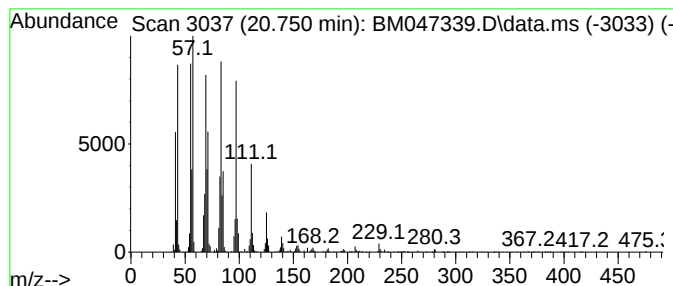
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 1-Heneicosanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.750	8.69 ng	1436280	Chrysene-d12	21.015

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosanol	312	C21H44O	015594-90-8	95
2			1-Tetracosene	336	C24H48	010192-32-2	94
3			1-Heptacosanol	396	C27H56O	002004-39-9	93
4			1-Hexacosanol	382	C26H54O	000506-52-5	91
5			Pentacos-1-ene	350	C25H50	016980-85-1	91



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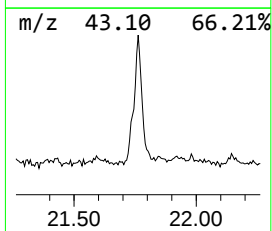
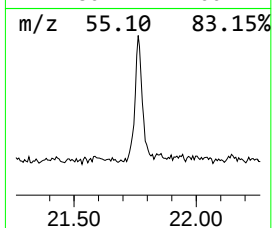
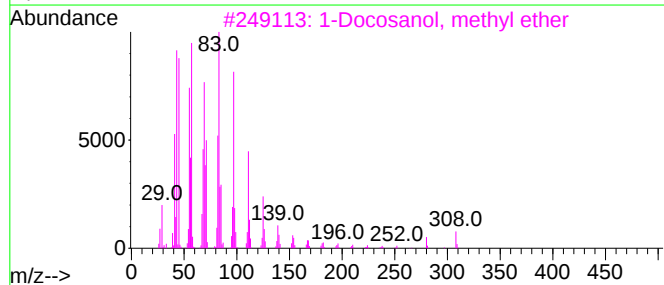
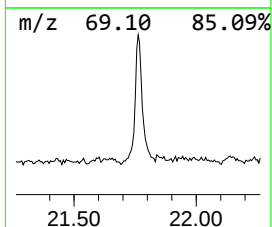
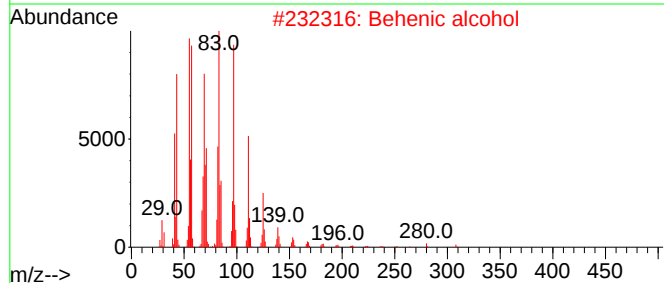
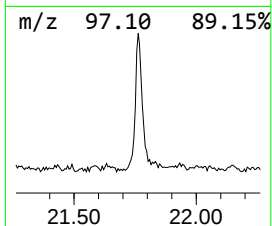
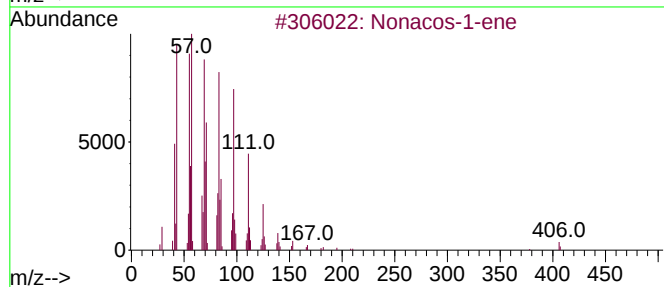
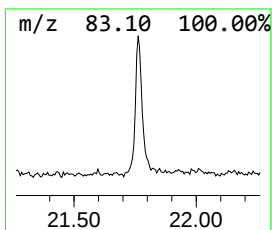
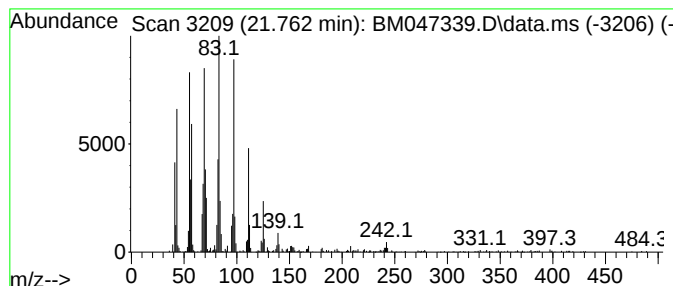
Instrument :
BNA_M
ClientSampleId :
SP-1-COMP

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

Peak Number 6 Nonacos-1-ene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.762	5.15 ng	851355	Chrysene-d12	21.015	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonacos-1-ene	406	C29H58	018835-35-3	91
2	Behenic alcohol	326	C22H46O	000661-19-8	90
3	1-Docosanol, methyl ether	340	C23H48O	1000333-91-9	90
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	90
5	Heptacos-1-ene	378	C27H54	015306-27-1	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082324\
Data File : BM047339.D
Acq On : 23 Aug 2024 18:47
Operator : RC/JU
Sample : P3640-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SP-1-COMP

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	3.257	3.9	ng	390744	1	7.351	1993720	20.0
2-Pentanone, 4-...	4.563	3.7	ng	370673	1	7.351	1993720	20.0
1-Phenoxypropan...	10.869	4.2	ng	545696	2	10.104	2622320	20.0
n-Hexadecanoic ...	17.715	6.4	ng	1235440	4	16.774	3856030	20.0
1-Heneicosanol	20.750	8.7	ng	1436280	5	21.015	3305120	20.0
Nonacos-1-ene	21.762	5.2	ng	851355	5	21.015	3305120	20.0