

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM060823\
 Data File : BM040178.D
 Acq On : 09 Jun 2023 04:09
 Operator : MA/JU
 Sample : 03047-07
 Misc :
 ALS Vial : 29 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 MW-41

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-BM060823.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM040178.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.534	376	382	391	rBV	1182337	1720282	18.07%	3.011%
2	7.139	648	655	666	rVB	758937	1180432	12.40%	2.066%
3	7.986	792	799	806	rBV	1115367	1735055	18.22%	3.037%
4	9.151	990	997	1008	rBV	1477954	2419814	25.41%	4.236%
5	10.804	1269	1278	1289	rBV	1506794	2563791	26.92%	4.488%
6	13.251	1687	1694	1713	rBV	4228796	5919156	62.16%	10.361%
7	14.627	1921	1928	1936	rBV	2299125	3352267	35.20%	5.868%
8	15.980	2153	2158	2172	rVB	1671067	2176292	22.85%	3.809%
9	16.109	2173	2180	2195	rBV	3314157	4502209	47.28%	7.881%
10	16.539	2249	2253	2259	rBV	130204	178072	1.87%	0.312%
11	17.368	2388	2394	2403	rBV	2970796	4056993	42.61%	7.101%
12	18.256	2540	2545	2553	rBV	811230	1233050	12.95%	2.158%
13	18.327	2554	2557	2569	rVB2	107593	205448	2.16%	0.360%
14	19.386	2733	2737	2739	rBV3	149084	205011	2.15%	0.359%
15	19.527	2757	2761	2771	rBV	415545	712442	7.48%	1.247%
16	19.756	2798	2800	2803	rVB2	125558	112664	1.18%	0.197%
17	19.792	2803	2806	2810	rVB	195448	212067	2.23%	0.371%
18	19.986	2833	2839	2844	rBV	7937200	9522207	100.00%	16.668%
19	20.291	2887	2891	2895	rVB	291281	344935	3.62%	0.604%
20	20.786	2971	2975	2979	rVB2	466670	520773	5.47%	0.912%
21	21.244	3049	3053	3060	rVB	1753545	2116902	22.23%	3.705%
22	21.544	3099	3104	3110	rBV	3662998	4801675	50.43%	8.405%
23	21.691	3126	3129	3133	rVB	632392	677476	7.11%	1.186%
24	22.156	3205	3208	3215	rBV	524946	821353	8.63%	1.438%
25	22.662	3291	3294	3300	rVB	387219	462071	4.85%	0.809%
26	23.979	3511	3518	3529	rBV	2629893	5377140	56.47%	9.412%

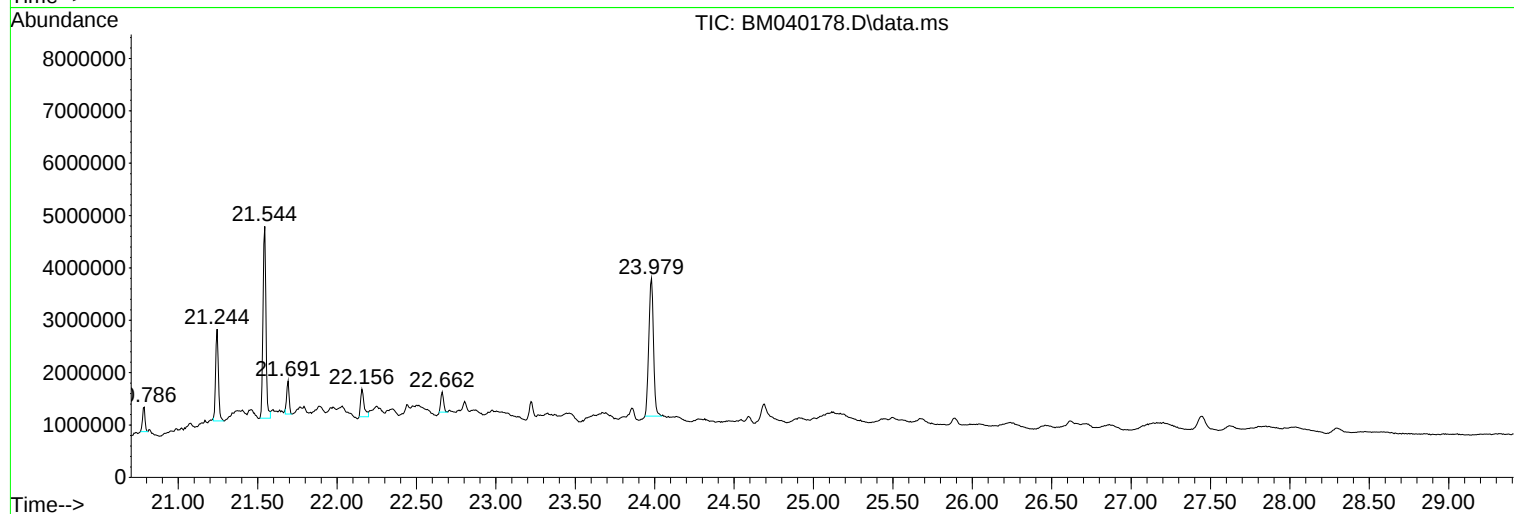
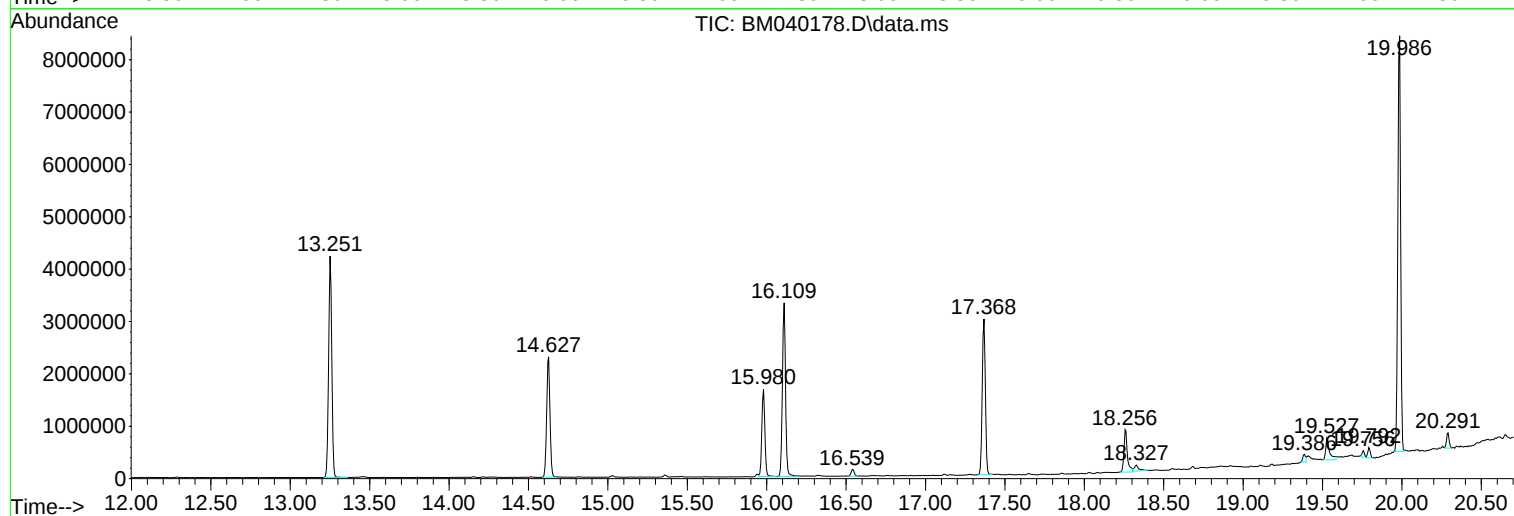
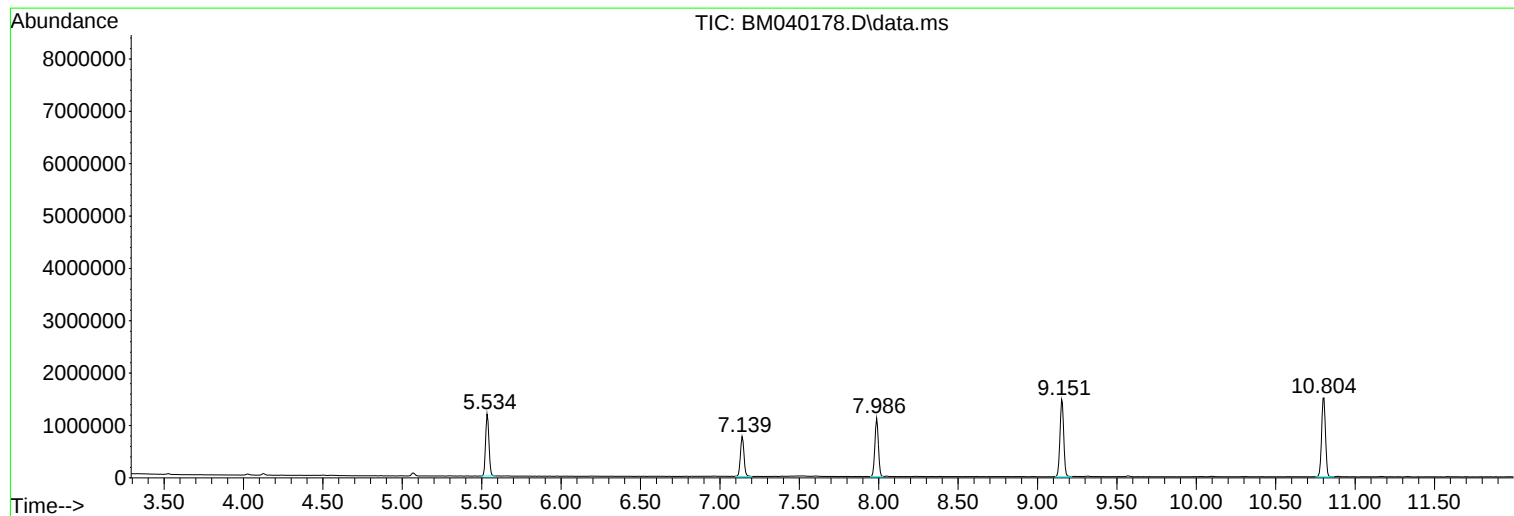
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM060823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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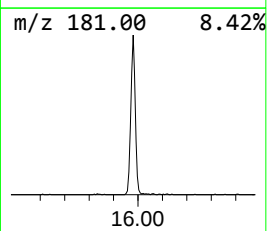
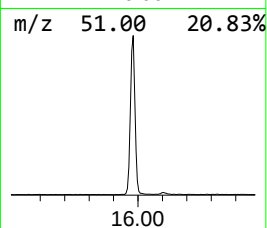
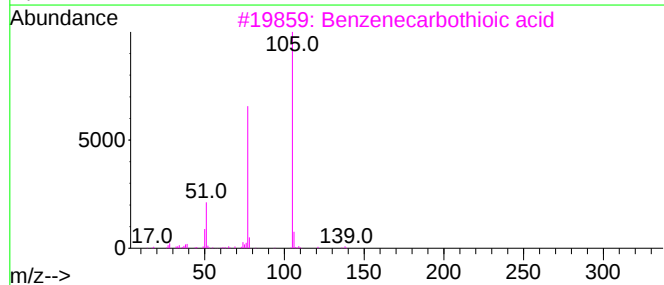
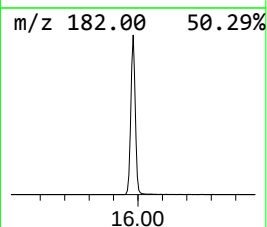
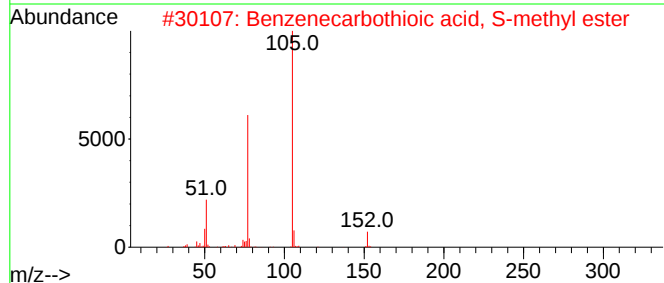
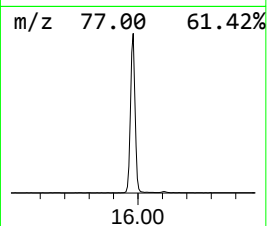
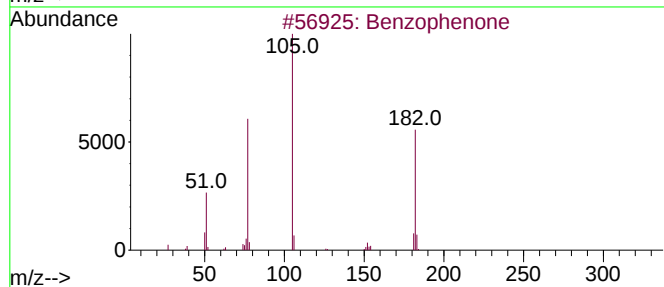
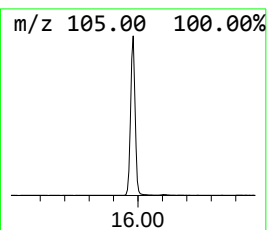
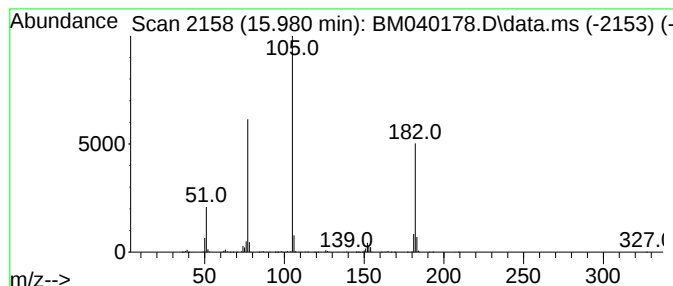
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TIC Library : C:\Database\NIST20.L
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Peak Number 1 Benzophenone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.980	12.98 ng	2176290	Acenaphthene-d10	14.627

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	50
3			Benzenecarbothioic acid	138	C7H6OS	000098-91-9	47
4			1,2-Propanedione, 1-phenyl-, 2-o...	163	C9H9NO2	000119-51-7	47
5			1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47



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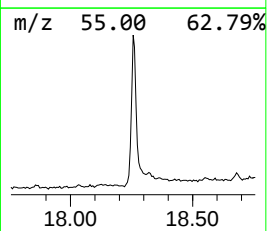
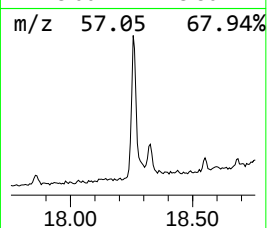
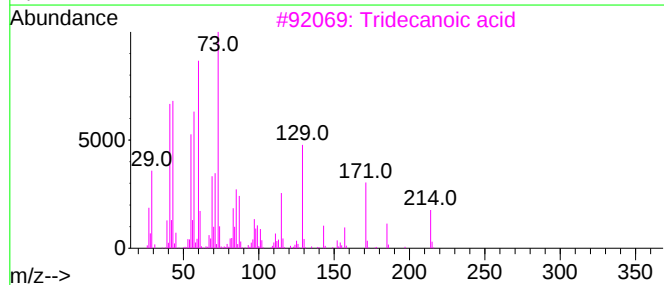
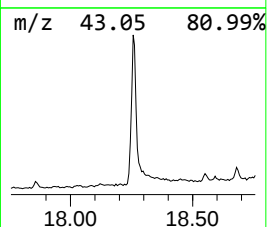
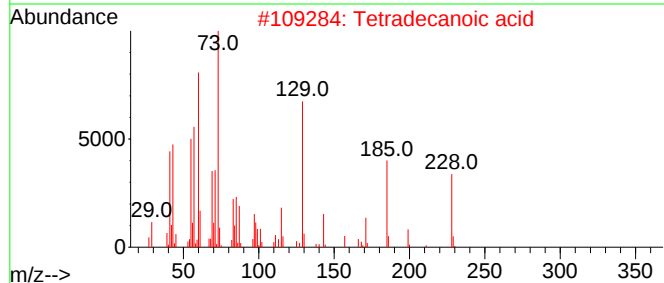
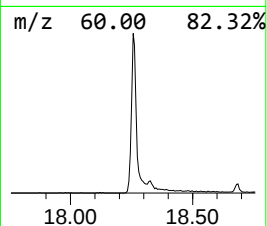
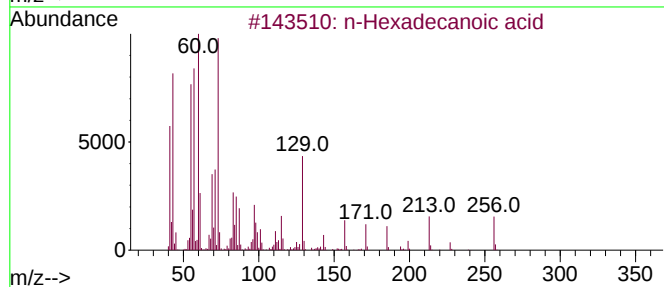
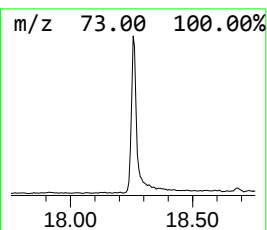
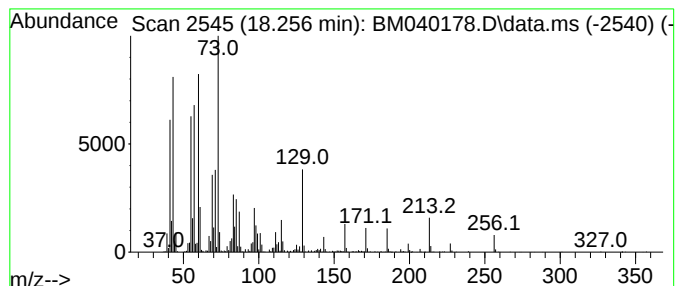
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.256	6.08 ng	1233050	Phenanthrene-d10	17.368

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	95
3		Tridecanoic acid	214	C13H26O2	000638-53-9	94
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	93
5		Octadecanoic acid	284	C18H36O2	000057-11-4	87



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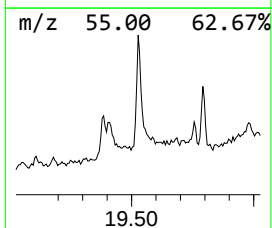
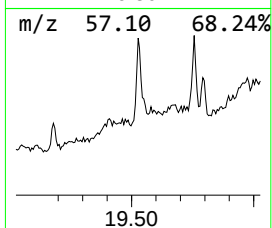
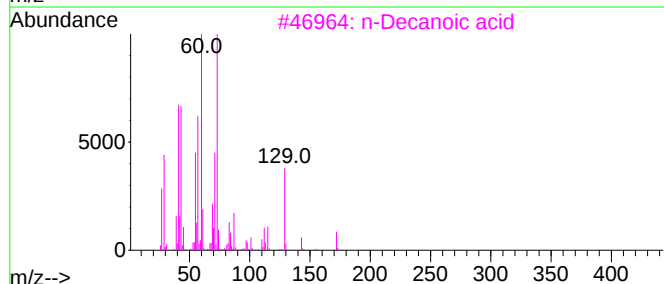
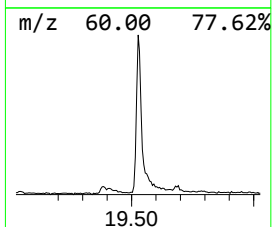
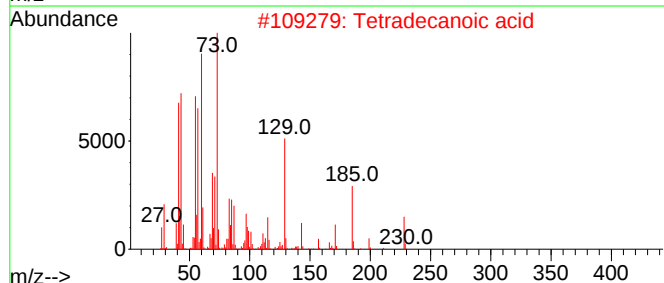
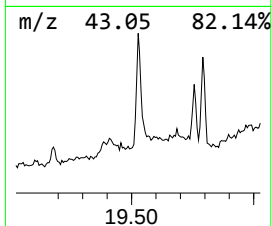
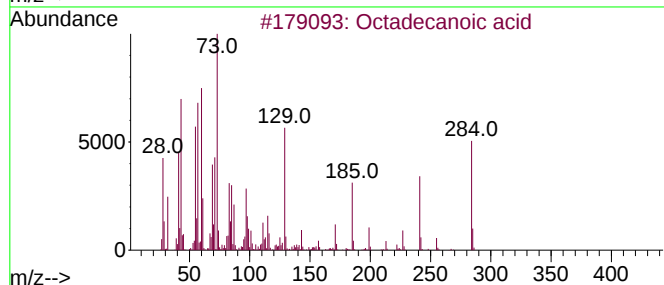
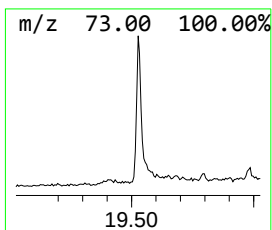
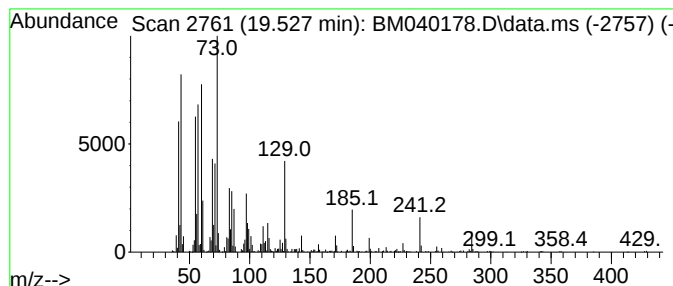
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Peak Number 3 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.527	2.97 ng	712442	Chrysene-d12	21.544

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	93
3			n-Decanoic acid	172	C10H20O2	000334-48-5	76
4			Tridecanoic acid	214	C13H26O2	000638-53-9	76
5			Ethanol, 2-(hexadecyloxy)-	286	C18H38O2	002136-71-2	20



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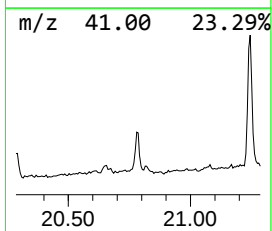
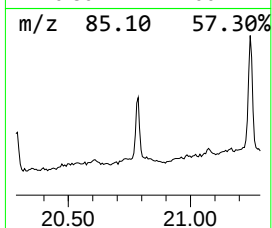
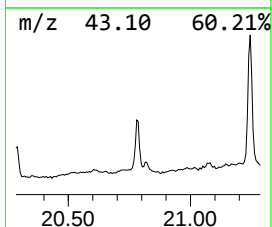
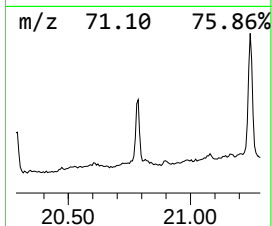
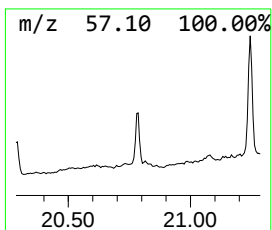
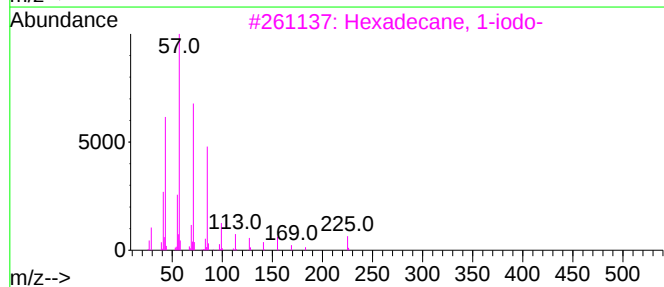
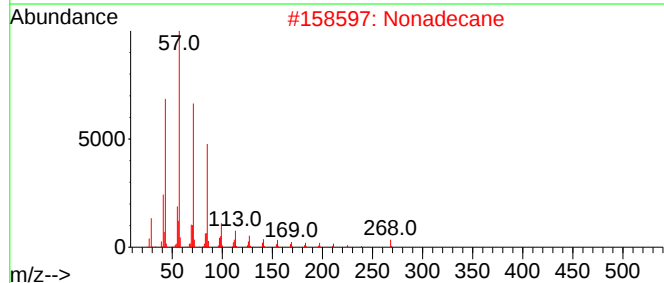
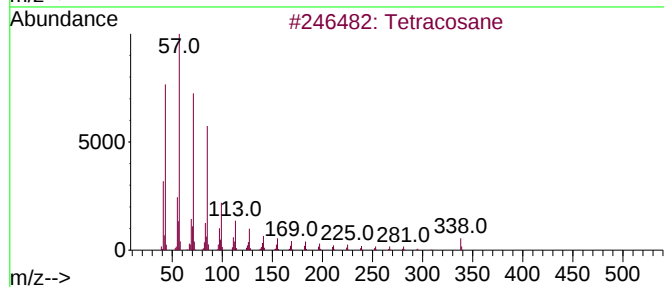
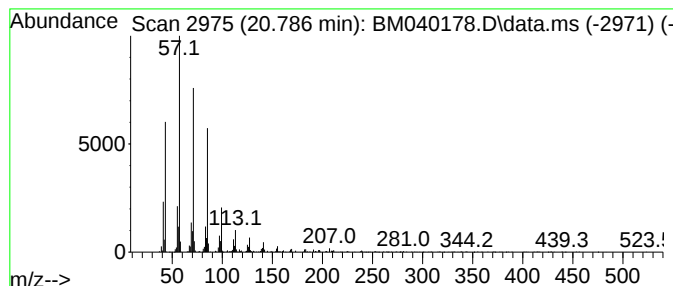
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Peak Number 4 Tetracosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
20.786	2.17 ng	520773	Chrysene-d12	21.544	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	97
2	Nonadecane	268	C19H40	000629-92-5	86
3	Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	86
4	Heneicosane	296	C21H44	000629-94-7	70
5	2-Bromo dodecane	248	C12H25Br	013187-99-0	68



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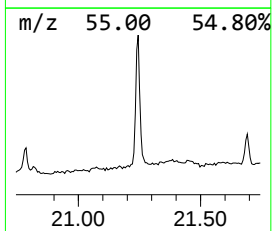
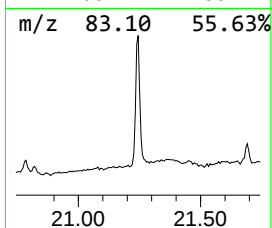
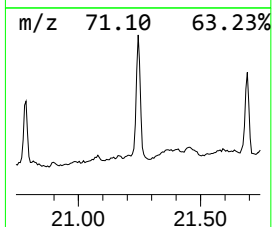
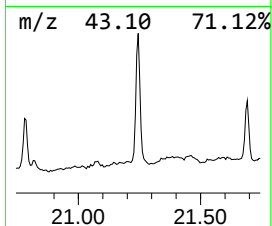
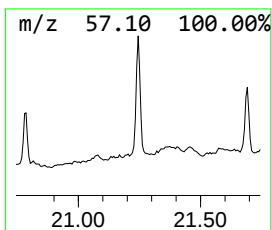
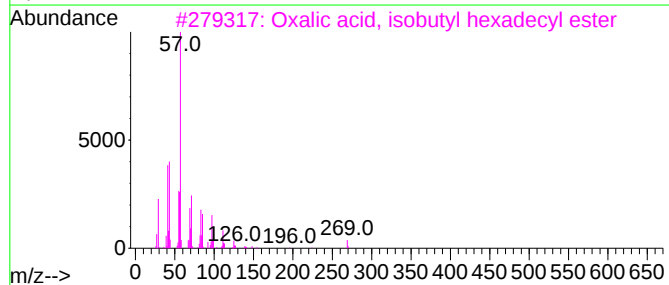
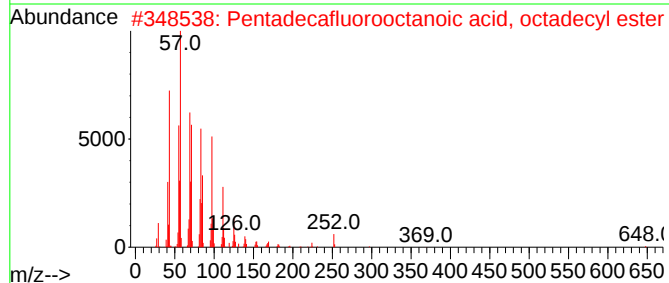
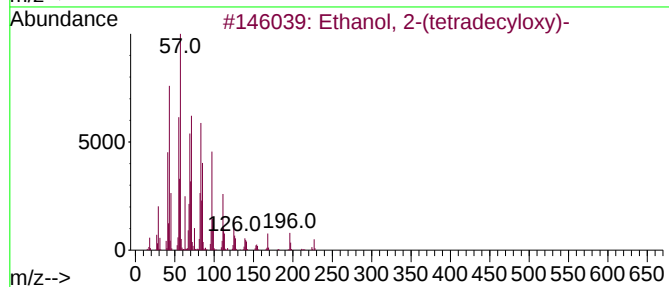
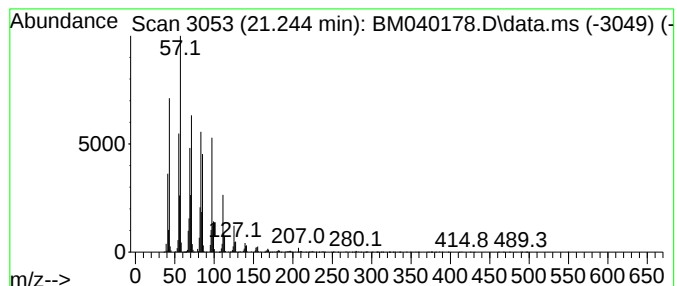
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Peak Number 5 Ethanol, 2-(tetradecyloxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.244	8.82 ng	2116900	Chrysene-d12	21.544	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	94
2	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	93
3	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	91
4	Oxalic acid, isobutyl tetradecyl...	342	C20H38O4	1000309-37-9	91
5	Cyclohexadecane	224	C16H32	000295-65-8	91



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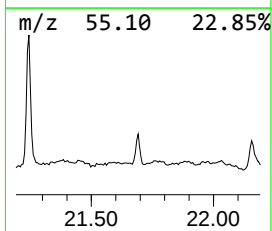
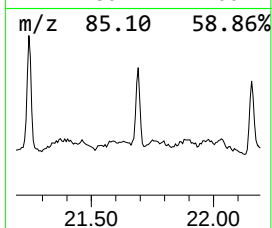
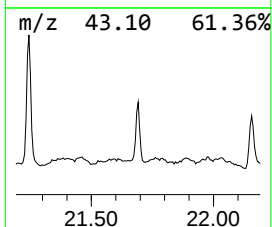
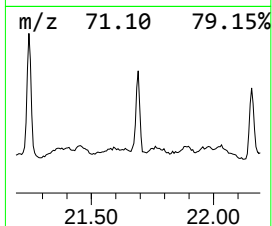
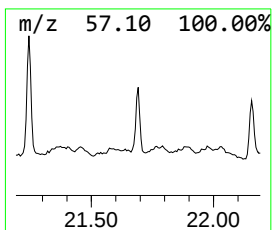
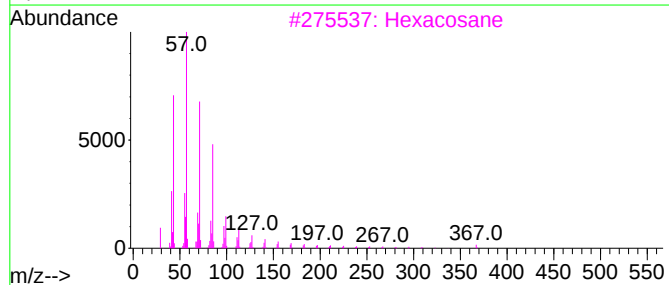
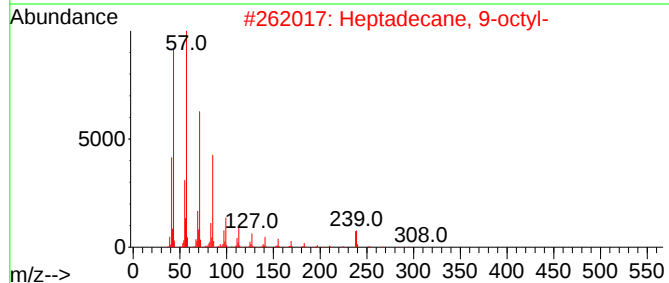
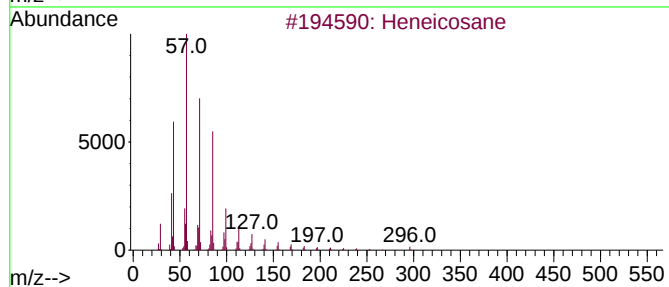
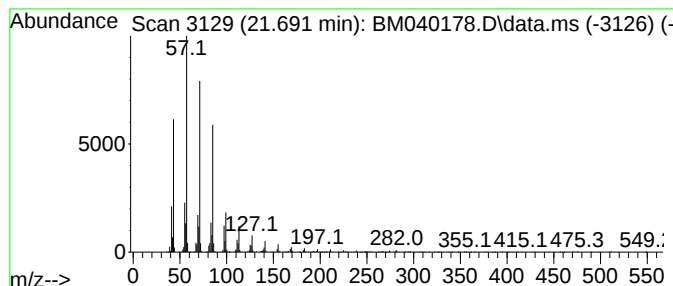
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.691	2.82 ng	677476	Chrysene-d12	21.544

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	91
2			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
3			Hexacosane	366	C26H54	000630-01-3	91
4			Heptadecane	240	C17H36	000629-78-7	91
5			Eicosane, 7-hexyl-	366	C26H54	055333-99-8	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM060823\
Data File : BM040178.D
Acq On : 09 Jun 2023 04:09
Operator : MA/JU
Sample : 03047-07
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MW-41

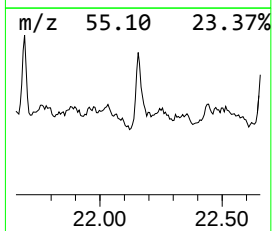
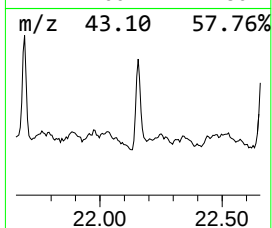
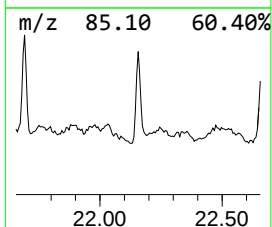
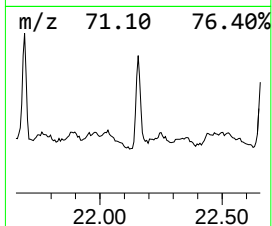
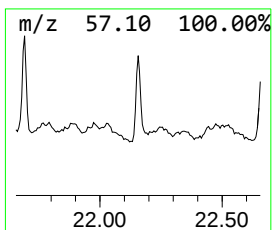
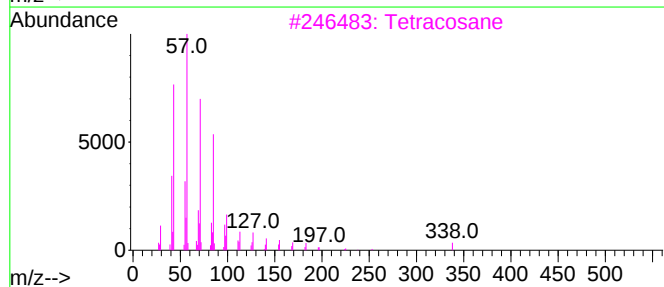
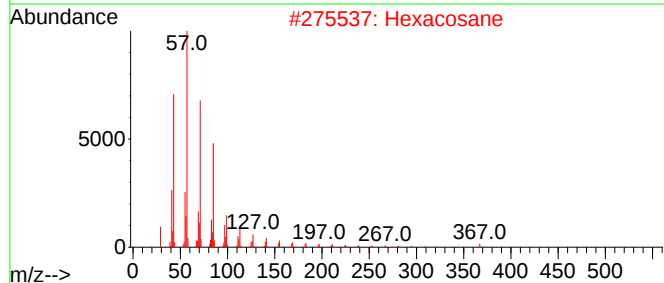
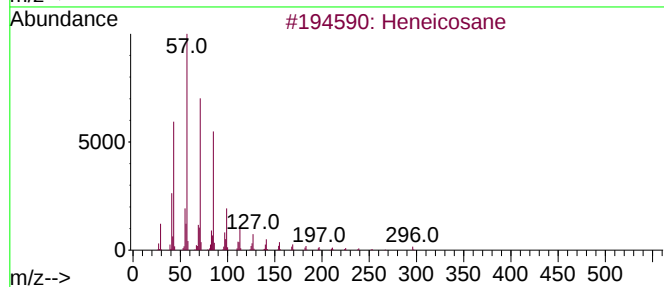
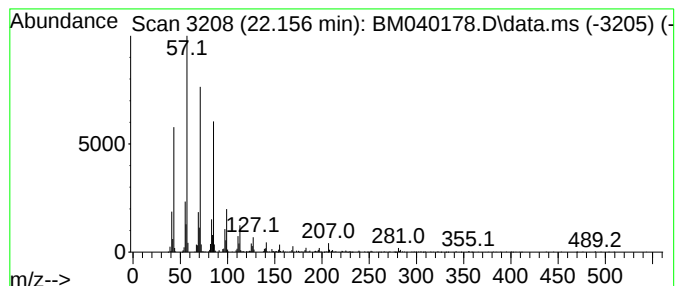
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.156	3.42 ng	821353	Chrysene-d12	21.544

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	90
2			Hexacosane	366	C26H54	000630-01-3	87
3			Tetracosane	338	C24H50	000646-31-1	87
4			Heptadecane	240	C17H36	000629-78-7	87
5			Eicosane	282	C20H42	000112-95-8	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM060823\
Data File : BM040178.D
Acq On : 09 Jun 2023 04:09
Operator : MA/JU
Sample : 03047-07
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MW-41

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM060823.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
Benzophenone	15.980	13.0	ng	2176290	3	14.627	3352270	20.0
n-Hexadecanoic ...	18.256	6.1	ng	1233050	4	17.368	4056990	20.0
Octadecanoic acid	19.527	3.0	ng	712442	5	21.544	4801680	20.0
Tetracosane	20.786	2.2	ng	520773	5	21.544	4801680	20.0
Ethanol, 2-(tet...	21.244	8.8	ng	2116900	5	21.544	4801680	20.0
Heneicosane	21.691	2.8	ng	677476	5	21.544	4801680	20.0
Hexacosane	22.156	3.4	ng	821353	5	21.544	4801680	20.0