

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM091824\
 Data File : BM047555.D
 Acq On : 18 Sep 2024 14:22
 Operator : RC/JU
 Sample : P4087-19
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 NB-614-COMP-04

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-BM091424.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM047555.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.951	313	317	325	rVB	217039	322156	4.42%	0.720%
2	5.416	390	396	409	rBV	3408805	4821670	66.15%	10.777%
3	7.004	658	666	674	rBV	3298126	4952228	67.94%	11.069%
4	7.845	802	809	816	rBV	830058	1297775	17.80%	2.901%
5	8.992	996	1004	1014	rBV	1799593	2910063	39.92%	6.504%
6	9.557	1095	1100	1106	rBV	49244	75358	1.03%	0.168%
7	10.639	1275	1284	1291	rBV	999860	1646444	22.59%	3.680%
8	13.098	1695	1702	1709	rBV	3721402	5116649	70.20%	11.436%
9	14.474	1929	1936	1948	rBV	1264693	1810554	24.84%	4.047%
10	15.827	2160	2166	2172	rBV	170886	237449	3.26%	0.531%
11	15.951	2181	2187	2208	rBV	2654504	3588427	49.23%	8.021%
12	16.345	2234	2254	2258	rBV4	188064	852721	11.70%	1.906%
13	17.209	2392	2401	2406	rBV	1431068	1957555	26.86%	4.375%
14	18.109	2547	2554	2563	rBV	708787	1099811	15.09%	2.458%
15	19.380	2766	2770	2780	rBV2	277923	379548	5.21%	0.848%
16	19.821	2840	2845	2857	rBV	6117888	7289059	100.00%	16.292%
17	21.121	3061	3066	3076	rBV2	248673	438597	6.02%	0.980%
18	21.433	3113	3119	3131	rBV	1464038	2153235	29.54%	4.813%
19	21.644	3153	3155	3162	rVB2	68161	92098	1.26%	0.206%
20	21.880	3187	3195	3203	rVB	532877	1384596	19.00%	3.095%
21	22.227	3251	3254	3262	rVB4	85821	146043	2.00%	0.326%
22	24.456	3625	3633	3645	rBV	891071	2168340	29.75%	4.846%

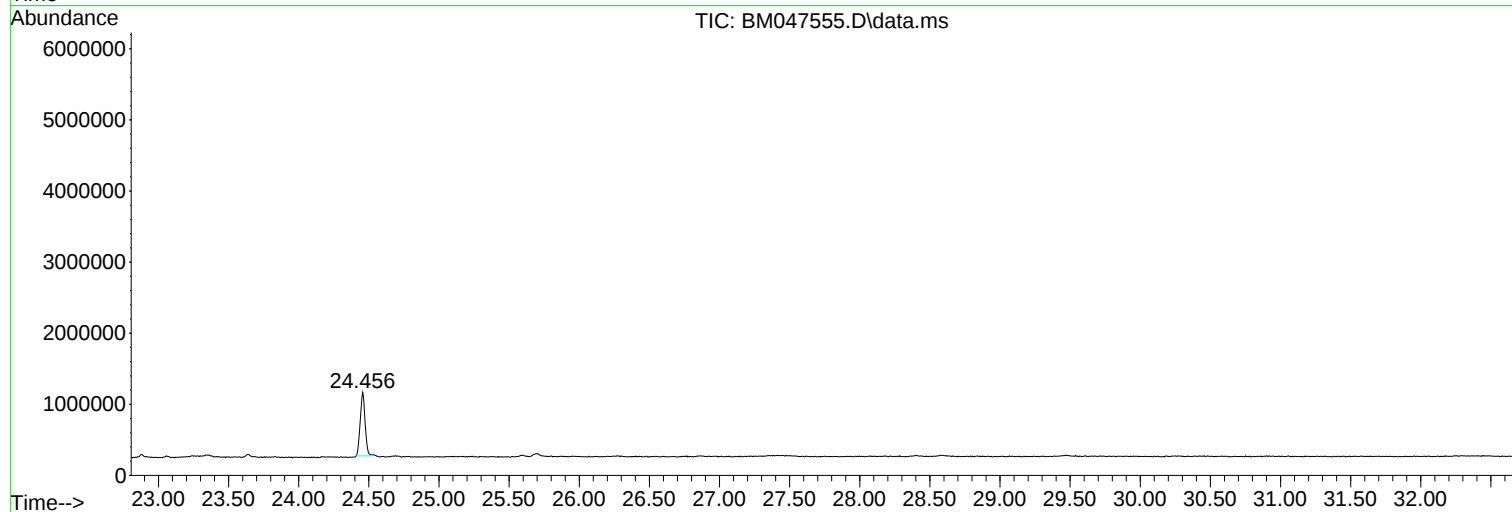
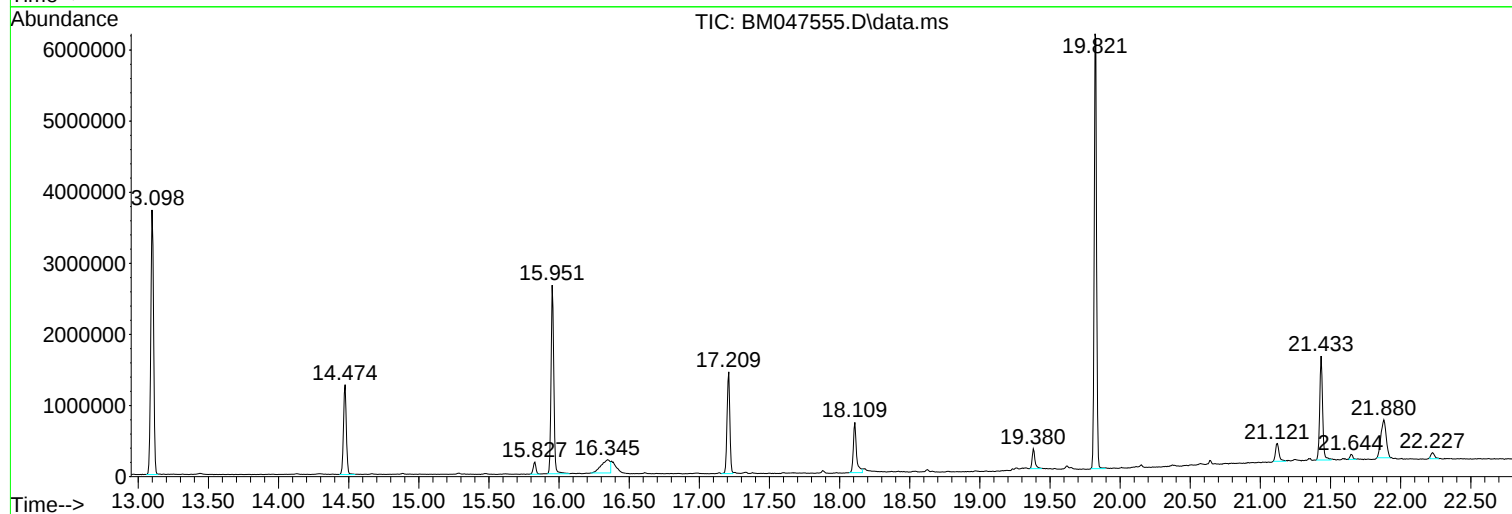
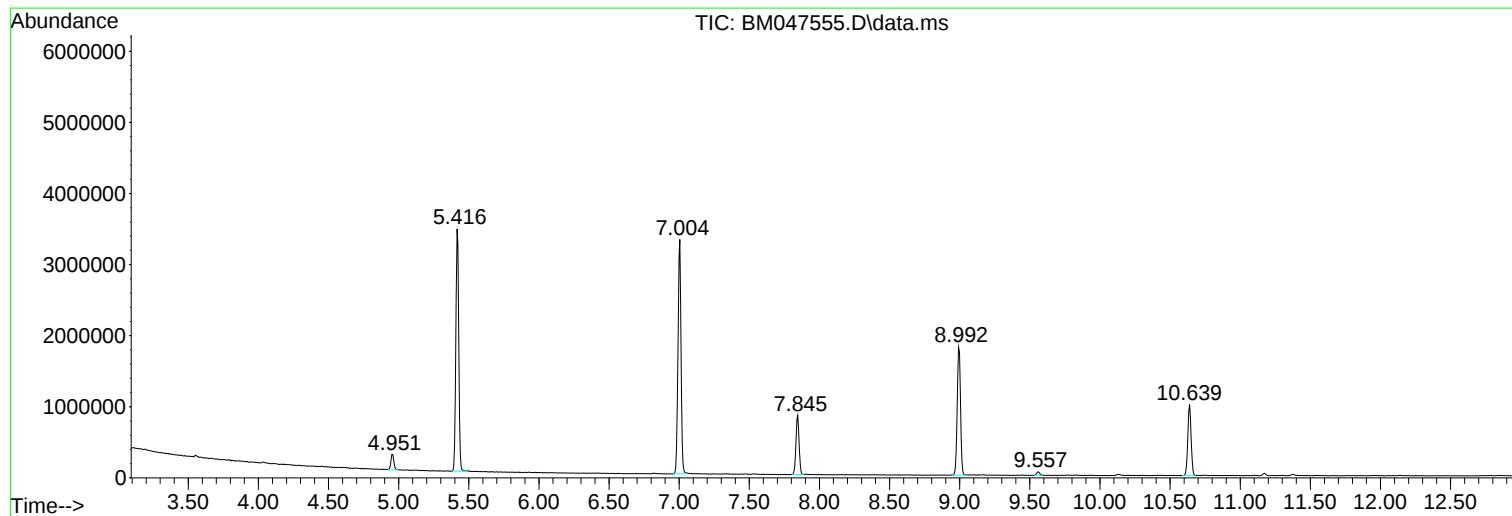
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM091424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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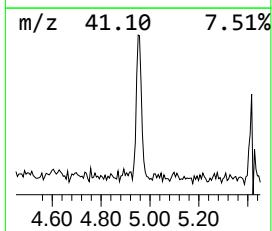
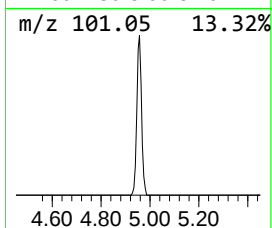
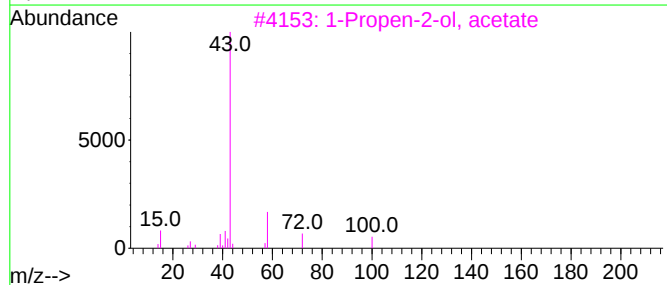
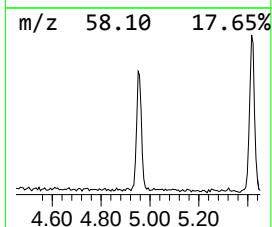
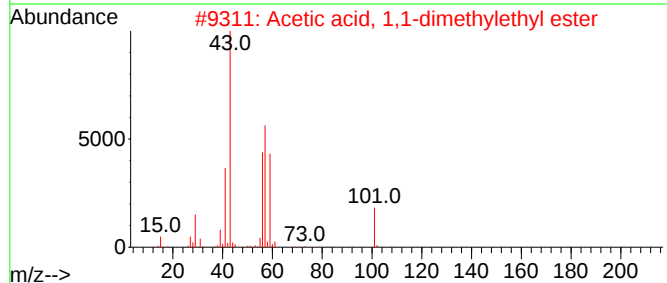
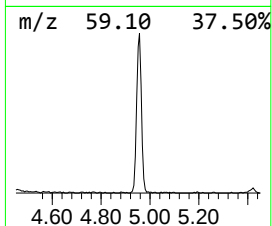
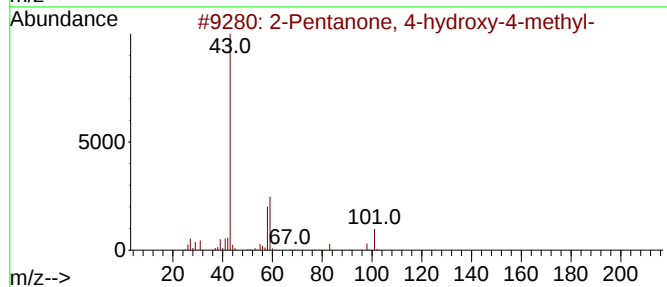
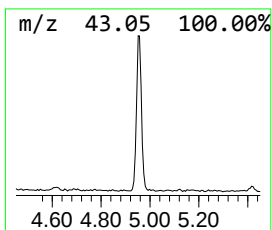
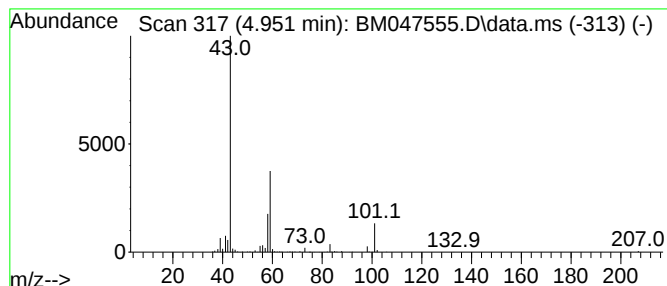
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.951	4.96 ng	322156	1,4-Dichlorobenzene-d4	7.845

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	78
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	42
3			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	16
4			Acetone	58	C3H6O	000067-64-1	9
5			N-(n-Propyl)acetamide	101	C5H11NO	005331-48-6	9



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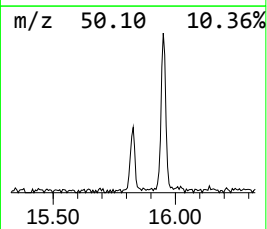
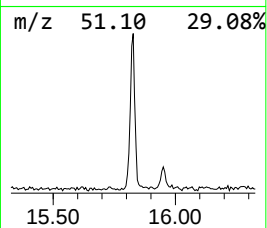
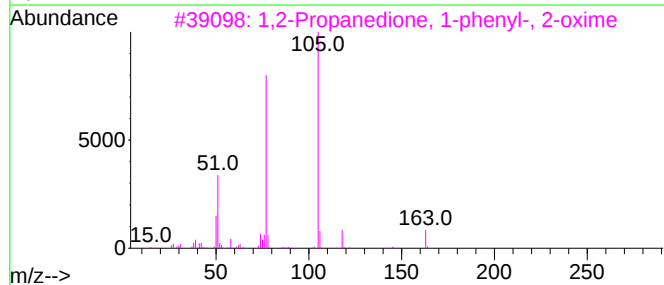
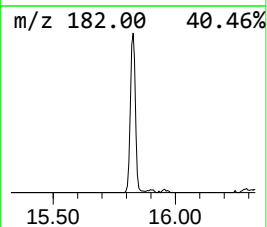
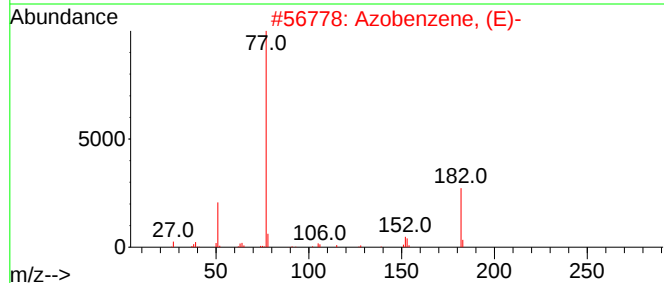
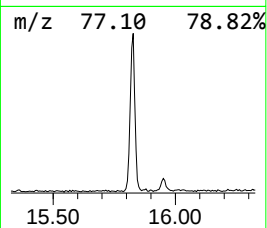
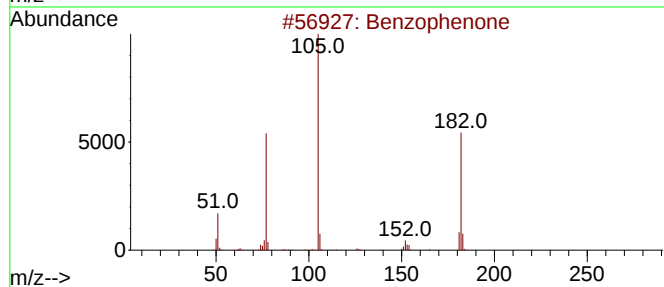
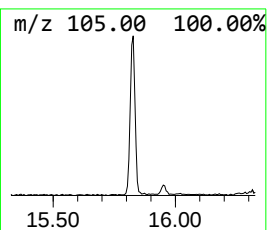
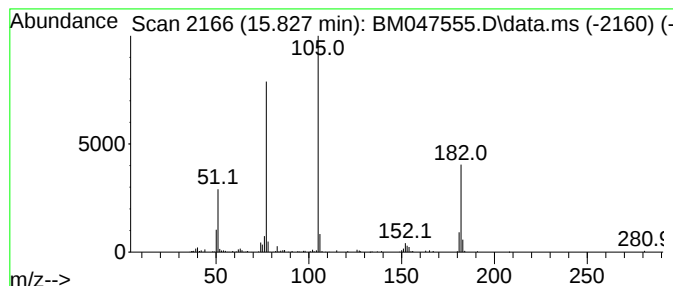
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Peak Number 2 Benzophenone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.827	2.62 ng	237449	Acenaphthene-d10	14.474

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			Azobenzene, (E)-	182	C12H10N2	017082-12-1	59
3			1,2-Propanedione, 1-phenyl-, 2-o...	163	C9H9NO2	000119-51-7	53
4			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	53
5			acetic acid, 2-bromo-, 2-oxo-2-p...	256	C10H9BrO3	1000401-50-0	53



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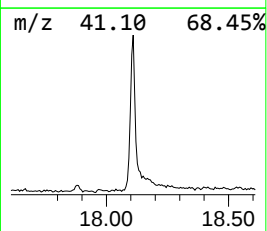
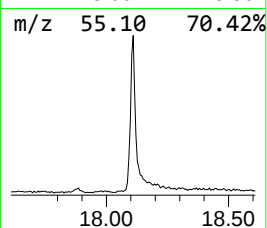
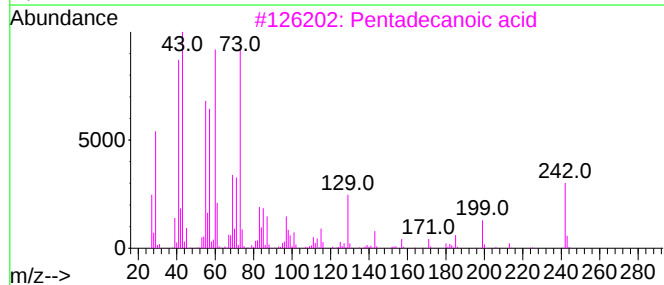
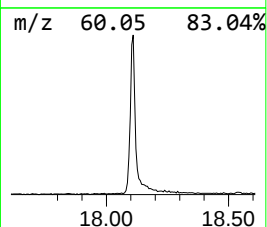
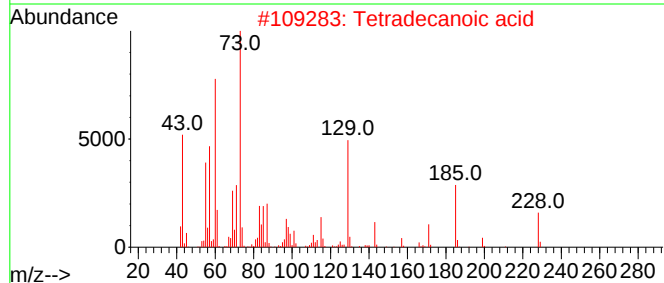
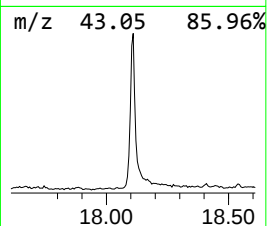
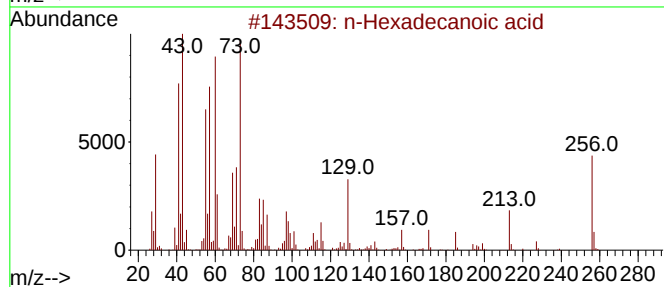
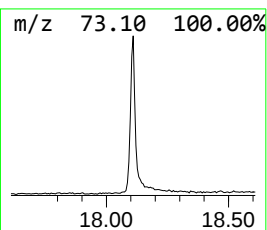
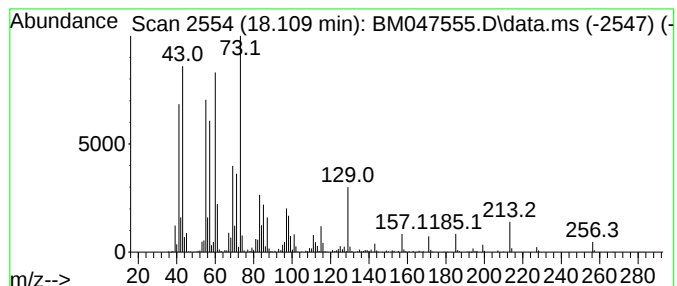
Instrument :
BNA_M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.109	11.24 ng	1099810	Phenanthrene-d10	17.209	
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	87
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
4	Dodecanoic acid	200	C12H24O2	000143-07-7	76
5	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	45



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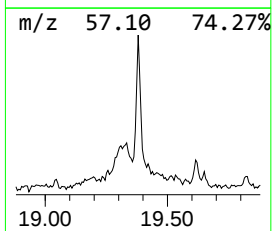
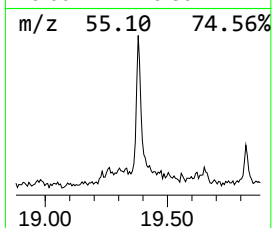
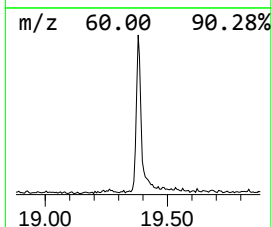
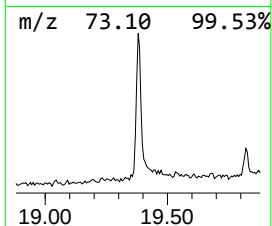
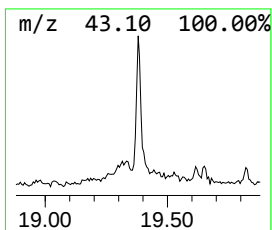
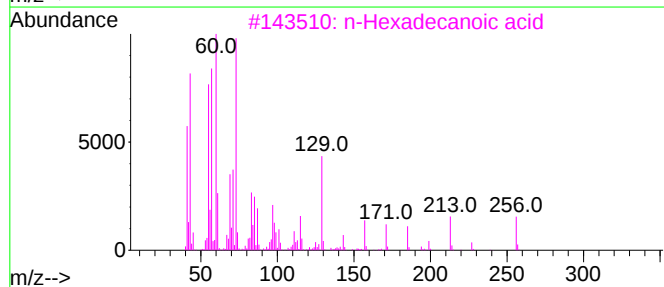
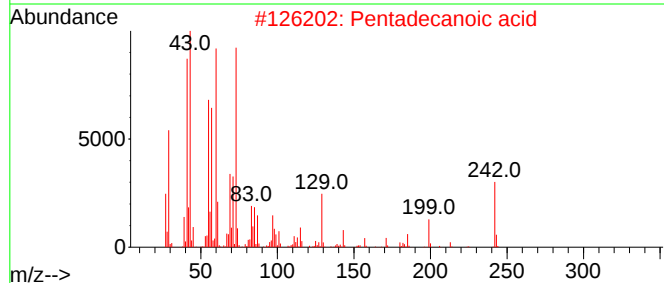
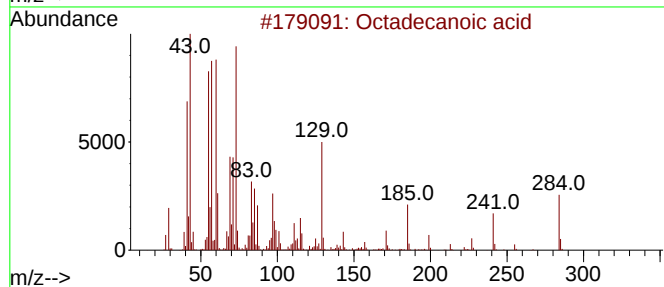
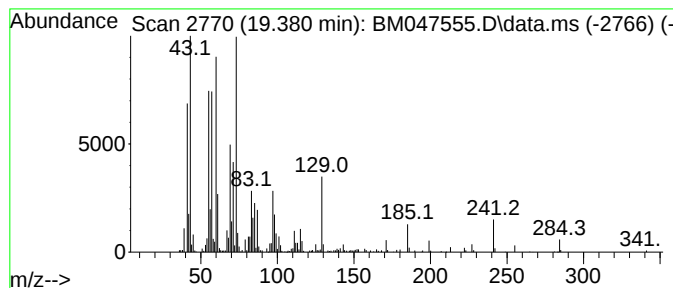
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Peak Number 5 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.380	3.53 ng	379548	Chrysene-d12	21.433

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
4			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	86
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	80



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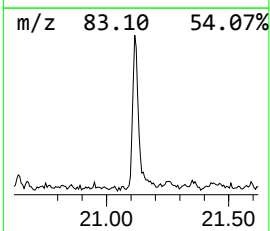
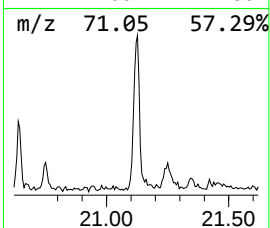
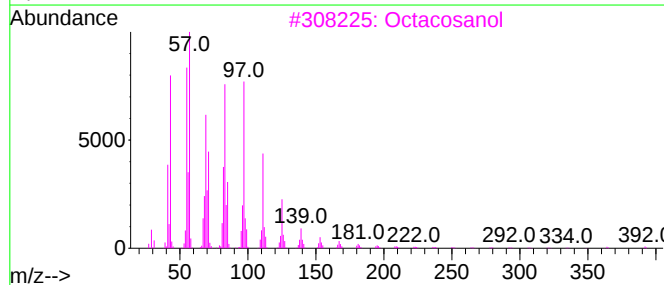
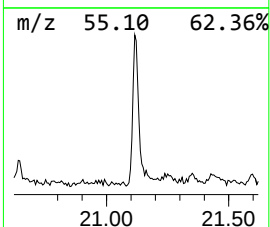
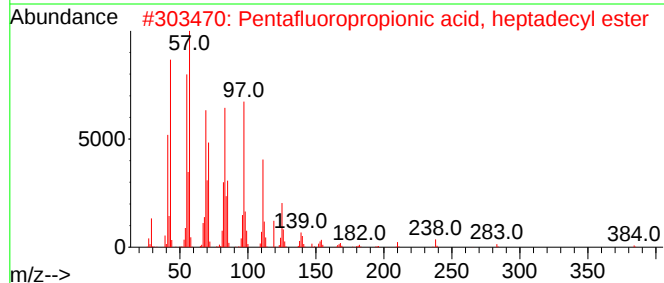
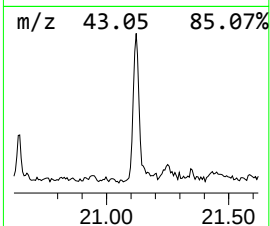
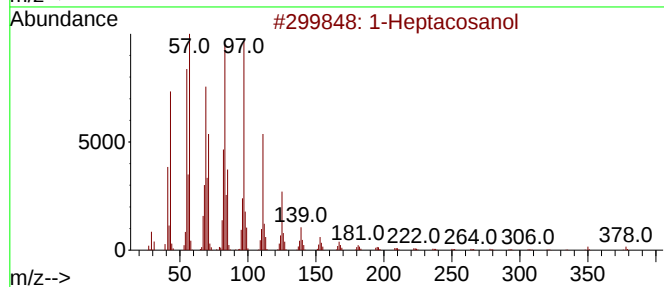
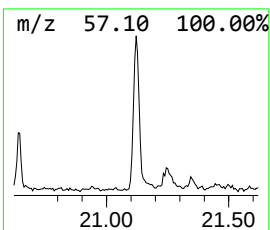
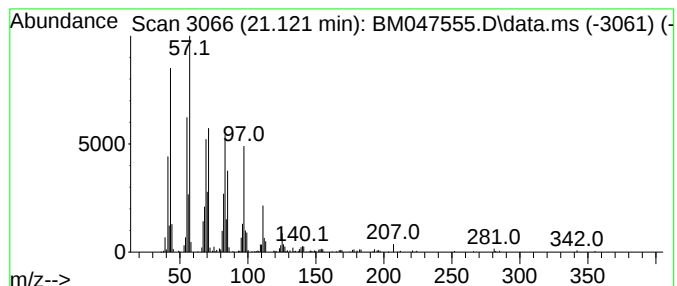
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 1-Heptacosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.121	4.07 ng	438597	Chrysene-d12	21.433

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heptacosanol	396	C27H56O	002004-39-9	90
2			Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	87
3			Octacosanol	410	C28H58O	000557-61-9	81
4			Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	81
5			Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	81



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.951	5.0	ng	322156	1	7.845	1297780	20.0
Benzophenone	15.827	2.6	ng	237449	3	14.474	1810550	20.0
n-Hexadecanoic ...	18.109	11.2	ng	1099810	4	17.209	1957560	20.0
Octadecanoic acid	19.380	3.5	ng	379548	5	21.433	2153240	20.0
1-Heptacosanol	21.121	4.1	ng	438597	5	21.433	2153240	20.0