

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081924\
 Data File : BM047257.D
 Acq On : 19 Aug 2024 18:08
 Operator : RC/JU
 Sample : P3609-02
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 920-J-WS-081424

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: BM047257.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.016	355	362	376	rBV	1156840	1751020	14.87%	3.980%
2	6.575	621	627	638	rVB	699970	1125376	9.56%	2.558%
3	7.363	755	761	769	rBV	586635	902706	7.67%	2.052%
4	8.510	949	956	966	rBV	1587941	2552078	21.68%	5.801%
5	10.116	1222	1229	1239	rBV	718279	1205120	10.24%	2.739%
6	10.880	1353	1359	1369	rBV	66660	134409	1.14%	0.305%
7	12.633	1648	1657	1670	rBV	3748791	5762461	48.95%	13.097%
8	13.904	1863	1873	1885	rBV2	60925	186974	1.59%	0.425%
9	14.021	1887	1893	1903	rVB	1109966	1648841	14.01%	3.748%
10	15.533	2143	2150	2171	rBV	4494285	6322860	53.71%	14.371%
11	16.786	2358	2363	2370	rBV	1513157	2091461	17.77%	4.754%
12	16.868	2372	2377	2382	rBV	177707	214934	1.83%	0.489%
13	17.727	2517	2523	2530	rBV	794687	1254390	10.66%	2.851%
14	19.027	2739	2744	2757	rBV	591690	987855	8.39%	2.245%
15	19.456	2811	2817	2822	rBV	9669333	11772699	100.00%	26.758%
16	20.768	3037	3040	3045	rVB3	123584	162300	1.38%	0.369%
17	21.027	3079	3084	3090	rBV2	2128188	2864287	24.33%	6.510%
18	23.732	3537	3544	3558	rVB	1273851	3056915	25.97%	6.948%

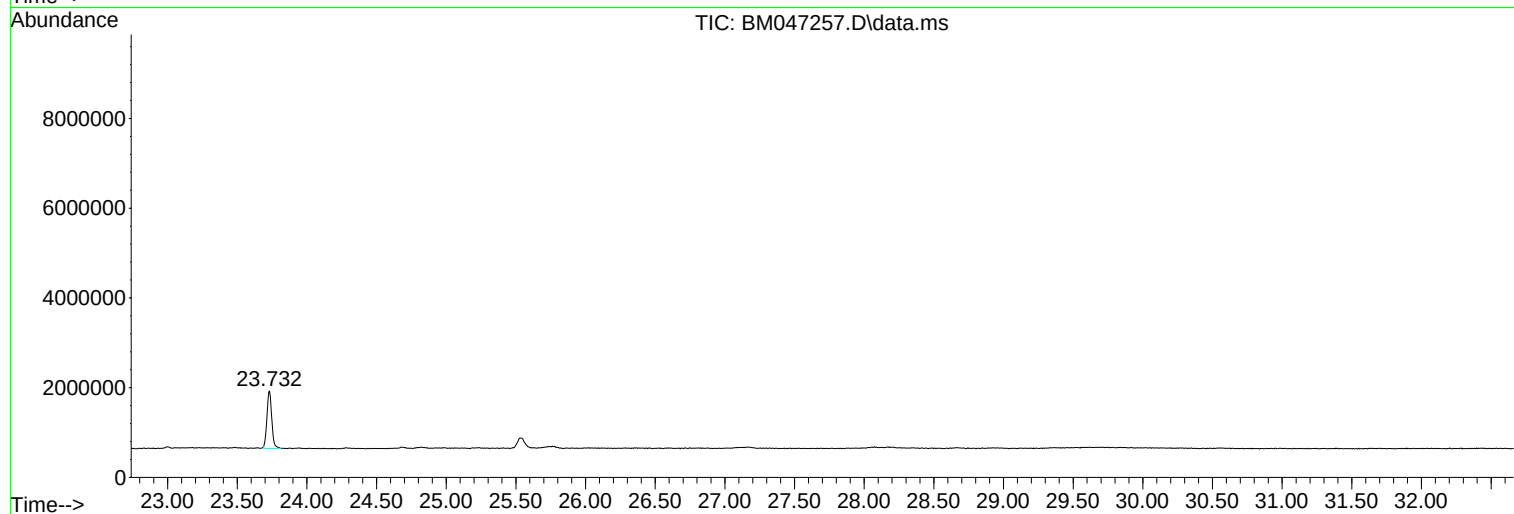
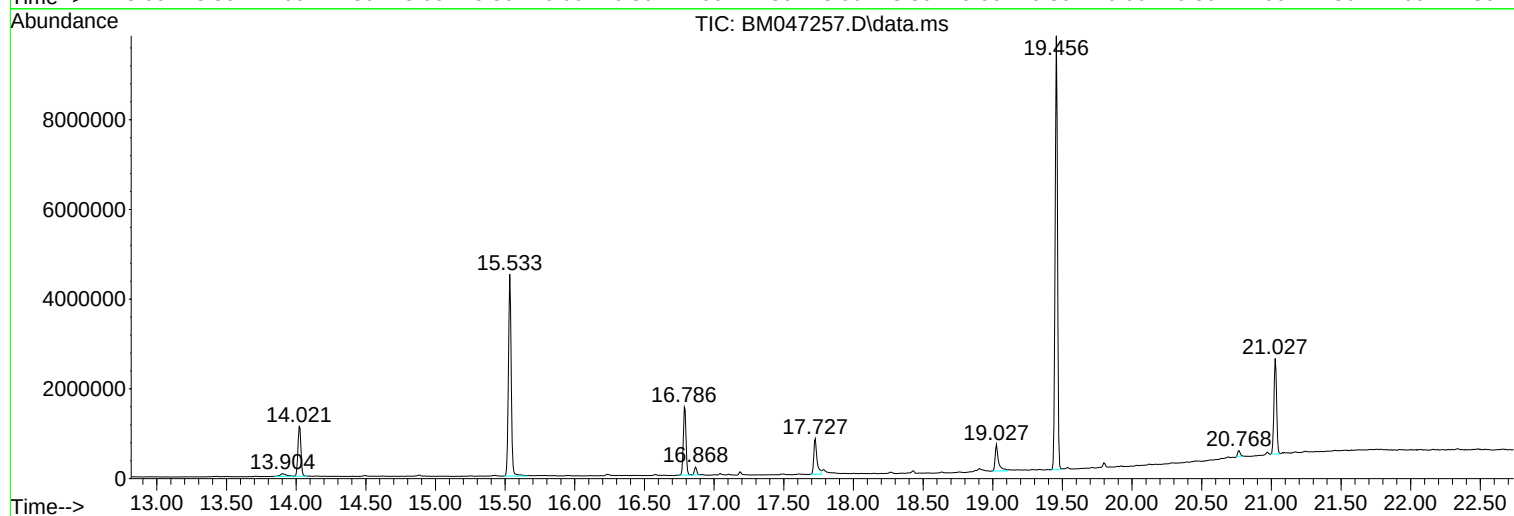
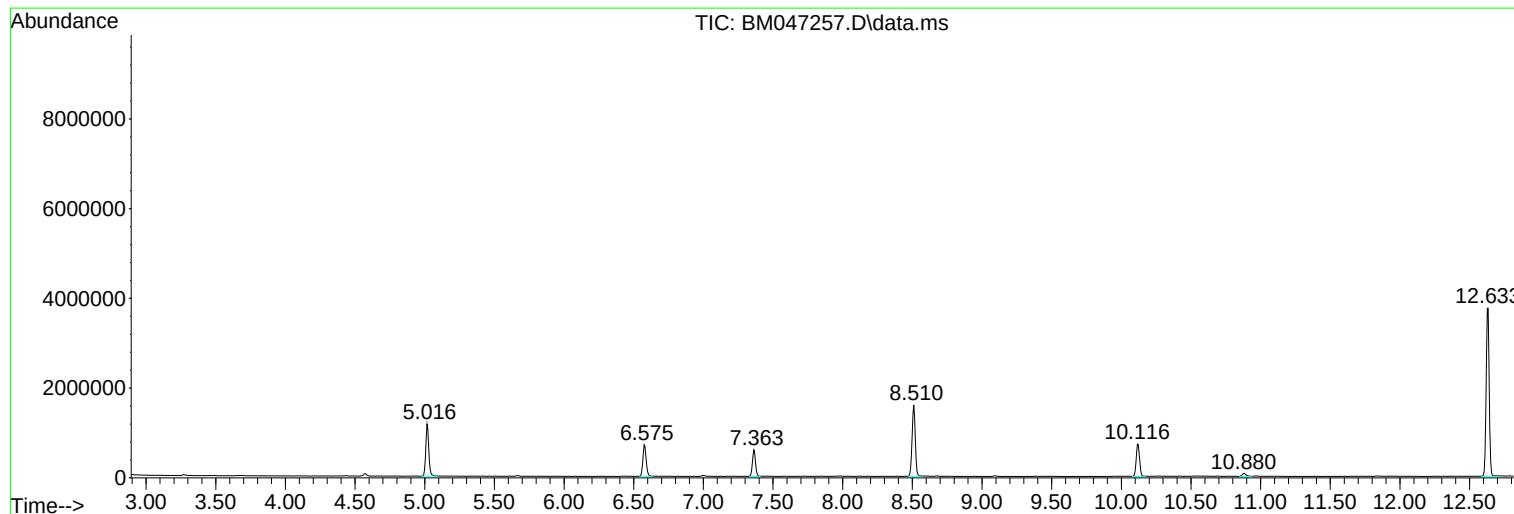
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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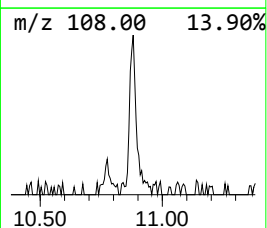
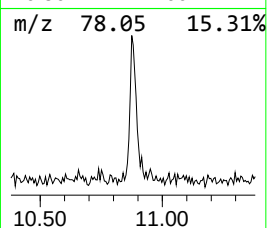
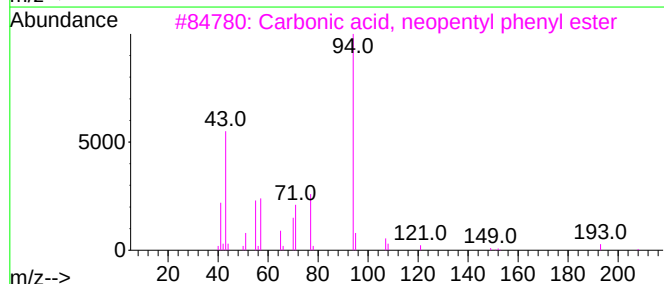
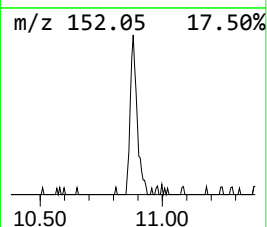
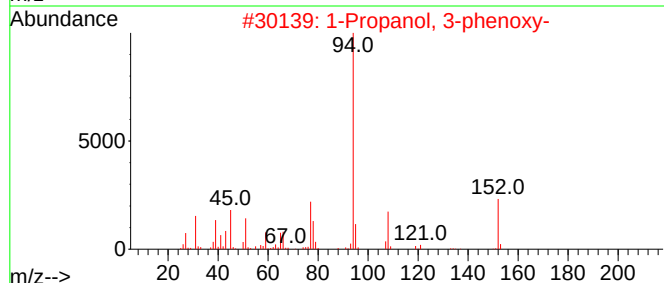
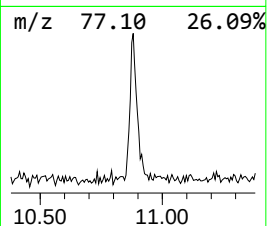
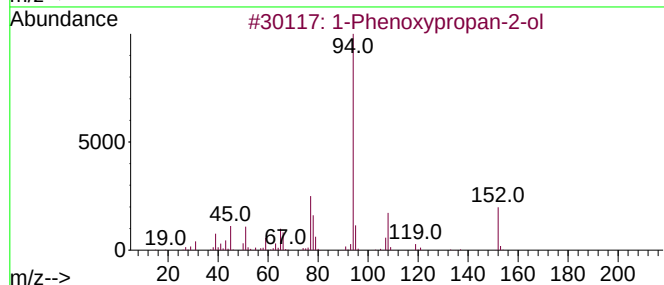
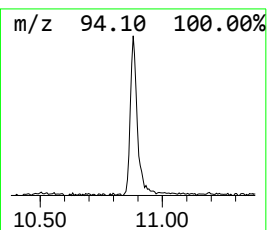
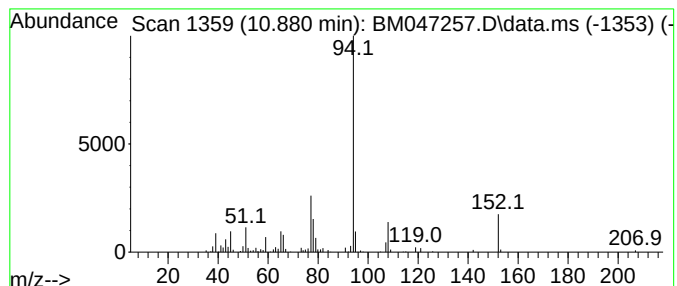
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 1-Phenoxypropan-2-ol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.880	2.23 ng	134409	Naphthalene-d8	10.116

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	94
2			1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	87
3			Carbonic acid, neopentyl phenyl ...	208	C12H16O3	013183-19-2	64
4			1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	59
5			Benzene, propoxy-	136	C9H12O	000622-85-5	53



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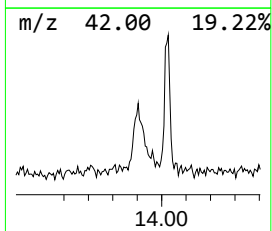
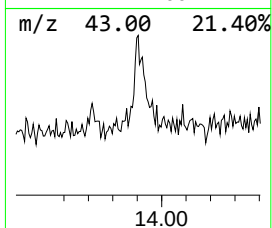
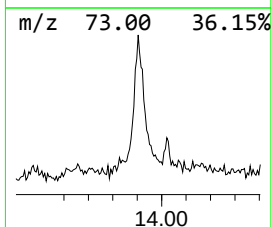
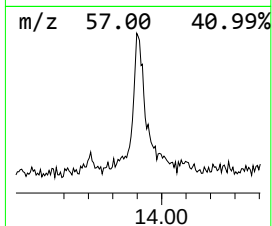
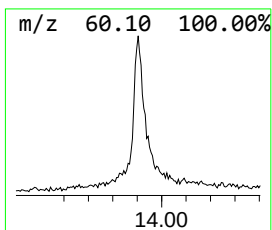
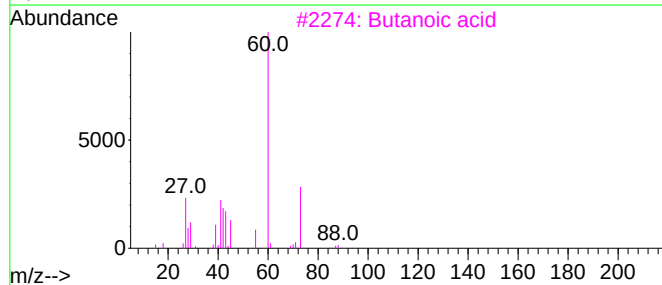
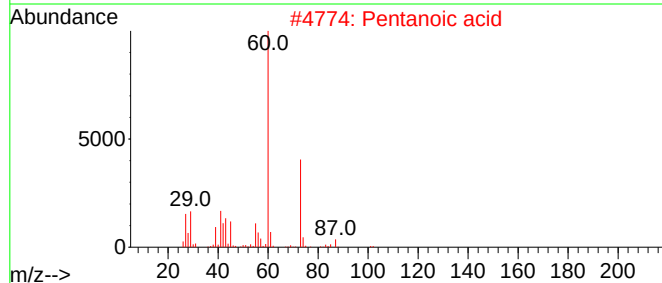
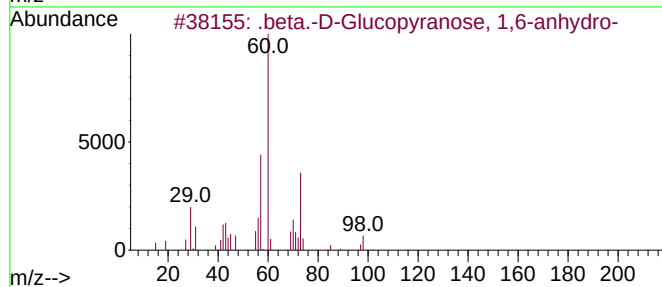
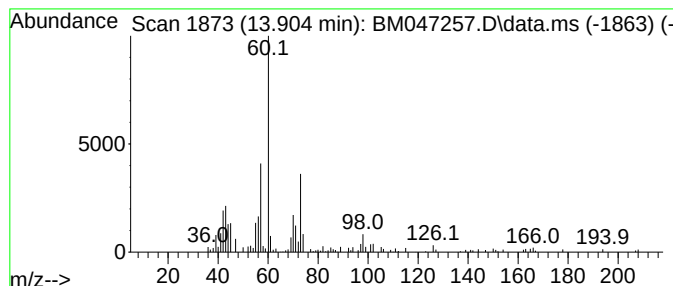
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Peak Number 2 .beta.-D-Glucopyranose, 1,6... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.904	2.27 ng	186974	Acenaphthene-d10	14.021

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		.beta.-D-Glucopyranose, 1,6-anhy...	162	C6H10O5	000498-07-7	72
2		Pentanoic acid	102	C5H10O2	000109-52-4	64
3		Butanoic acid	88	C4H8O2	000107-92-6	64
4		Ethyl .alpha.-d-glucopyranoside	208	C8H16O6	019467-01-7	56
5		Hexanoic acid	116	C6H12O2	000142-62-1	53



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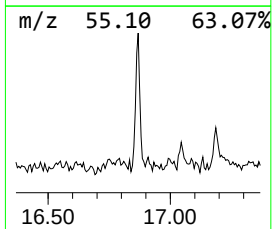
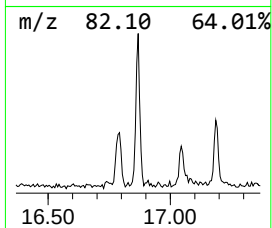
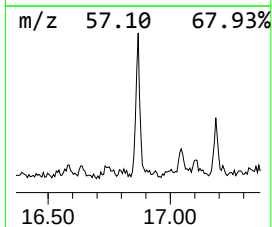
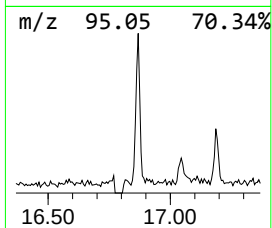
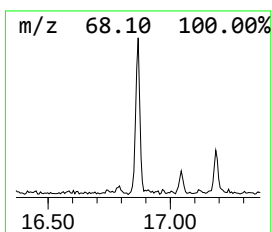
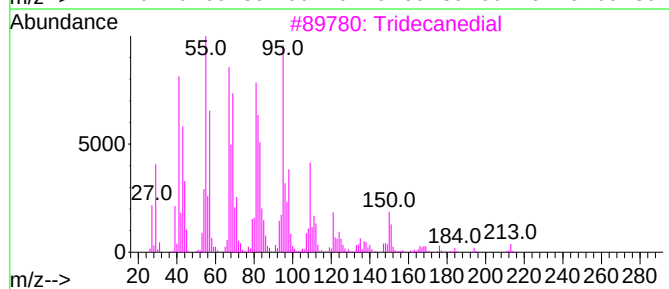
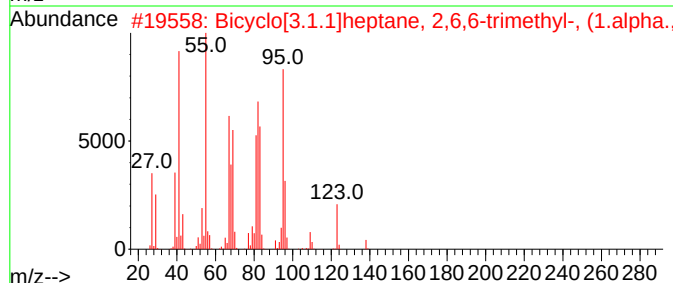
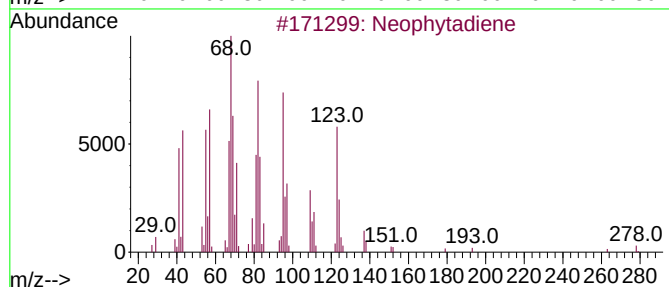
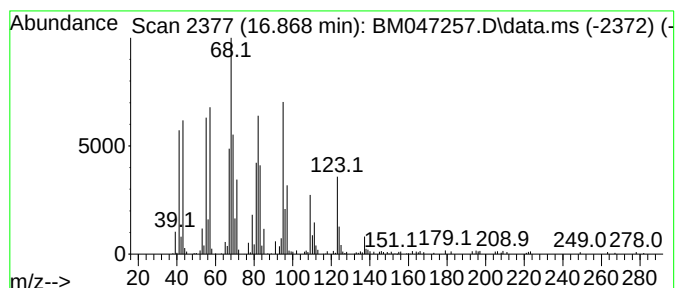
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Peak Number 3 Neophytadiene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.868	2.06 ng	214934	Phenanthrene-d10	16.786	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Neophytadiene	278	C20H38	000504-96-1	91
2	Bicyclo[3.1.1]heptane, 2,6,6-tri...	138	C10H18	006876-13-7	64
3	Tridecanedial	212	C13H24O2	063521-76-6	50
4	7-Octen-1-ol, 2,6-dimethyl-	156	C10H20O	157615-34-4	49
5	2-C14H26	194	C14H26	000638-60-8	43



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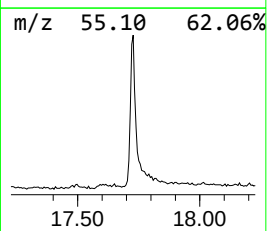
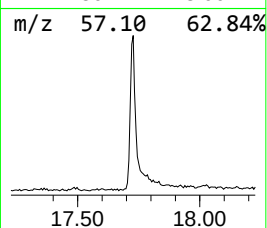
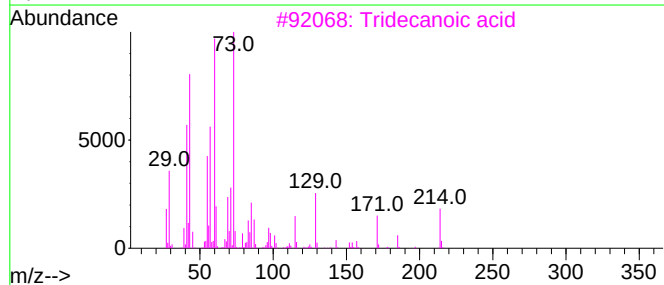
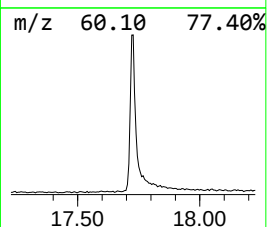
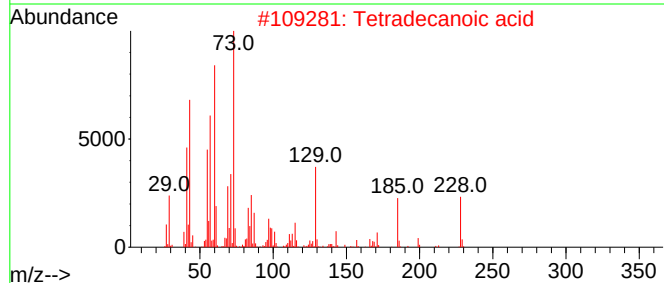
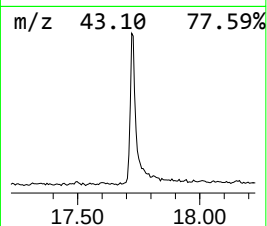
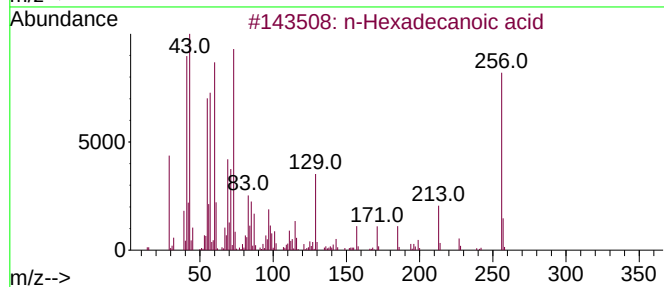
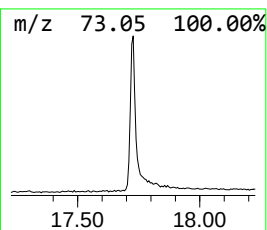
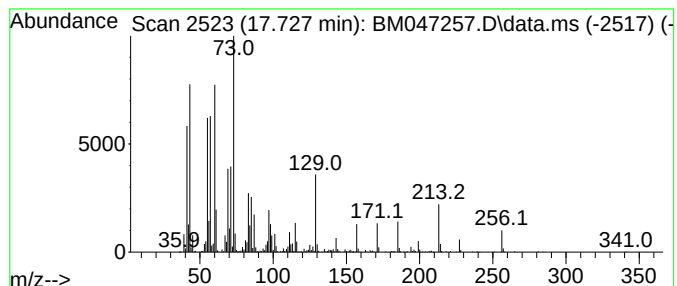
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.727	12.00 ng	1254390	Phenanthrene-d10	16.786

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	91
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5			Octadecanoic acid	284	C18H36O2	000057-11-4	87



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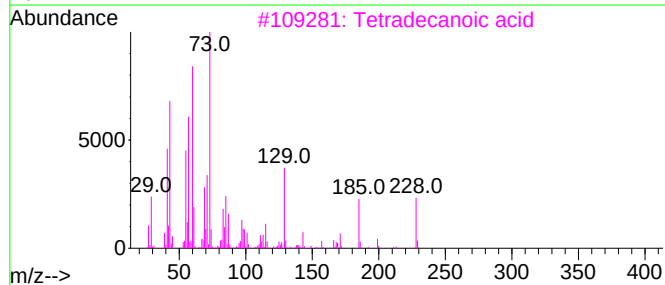
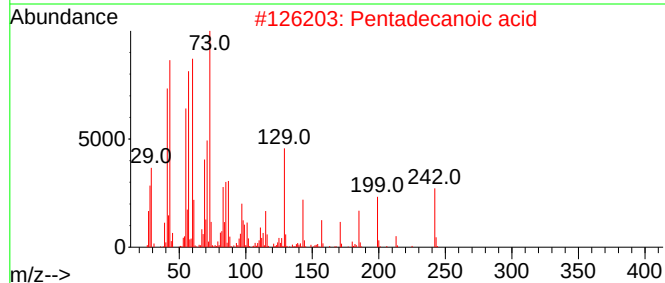
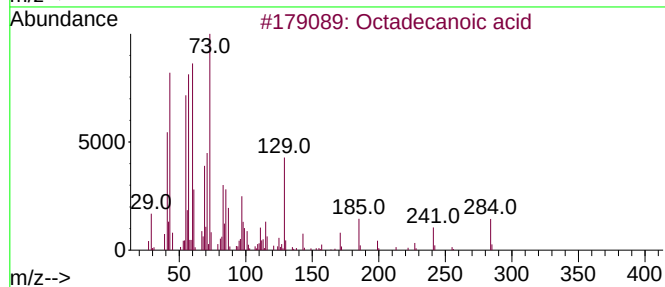
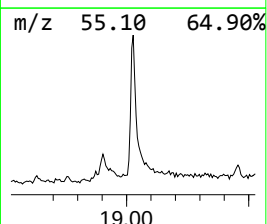
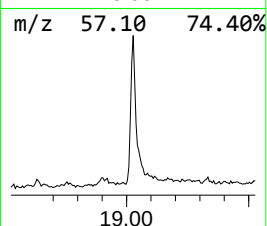
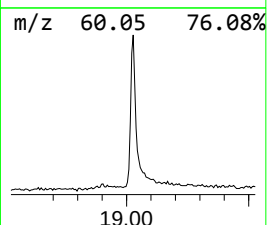
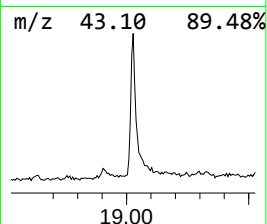
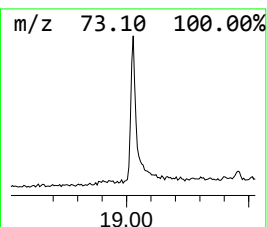
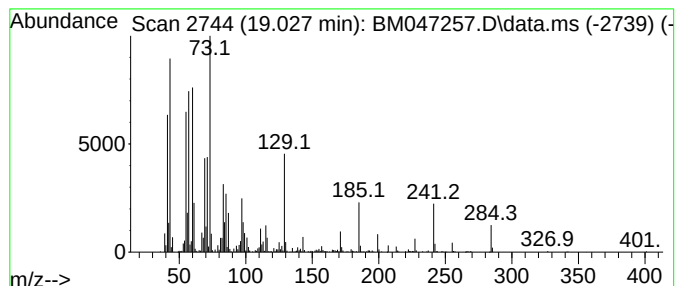
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Peak Number 5 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.027	6.90 ng	987855	Chrysene-d12	21.027

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	83
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	72
5			Tridecanoic acid	214	C13H26O2	000638-53-9	62



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1-Phenoxypropan...	10.880	2.2	ng	134409	2	10.116	1205120	20.0
.beta.-D-Glucop...	13.904	2.3	ng	186974	3	14.021	1648840	20.0
Neophytadiene	16.868	2.1	ng	214934	4	16.786	2091460	20.0
n-Hexadecanoic ...	17.727	12.0	ng	1254390	4	16.786	2091460	20.0
Octadecanoic acid	19.027	6.9	ng	987855	5	21.027	2864290	20.0