

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM021523\
 Data File : BM038752.D
 Acq On : 15 Feb 2023 17:37
 Operator : CG/JU
 Sample : 01539-09
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 COMP-8

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-BM020123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM038752.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.981	298	305	314	rBV	244307	337952	13.23%	2.389%
2	5.451	379	385	395	rBV	715786	1017733	39.85%	7.194%
3	7.069	653	660	670	rBV	691025	1066822	41.77%	7.541%
4	7.892	793	800	808	rBV	252042	379255	14.85%	2.681%
5	9.069	992	1000	1012	rBV	413546	664142	26.00%	4.694%
6	10.704	1271	1278	1285	rBV	315420	512664	20.07%	3.624%
7	13.163	1689	1696	1704	rBV	1339054	1840158	72.05%	13.007%
8	14.539	1923	1930	1937	rBV	521929	752015	29.45%	5.315%
9	15.898	2153	2161	2167	rBV	58020	75022	2.94%	0.530%
10	16.027	2176	2183	2196	rBV	1181786	1549384	60.67%	10.951%
11	17.280	2390	2396	2401	rBV	637980	852875	33.39%	6.028%
12	17.321	2401	2403	2409	rVB	39709	46566	1.82%	0.329%
13	18.162	2540	2546	2558	rBV	169009	279505	10.94%	1.976%
14	19.333	2740	2745	2754	rVB	102776	148568	5.82%	1.050%
15	19.439	2759	2763	2770	rBV2	83720	119193	4.67%	0.842%
16	19.698	2803	2807	2815	rVB	90222	119810	4.69%	0.847%
17	19.898	2836	2841	2847	rBV	2216523	2553930	100.00%	18.052%
18	21.150	3050	3054	3064	rBV3	130407	199112	7.80%	1.407%
19	21.456	3100	3106	3111	rBV	690191	915270	35.84%	6.469%
20	23.838	3504	3511	3517	rBV2	365931	717730	28.10%	5.073%

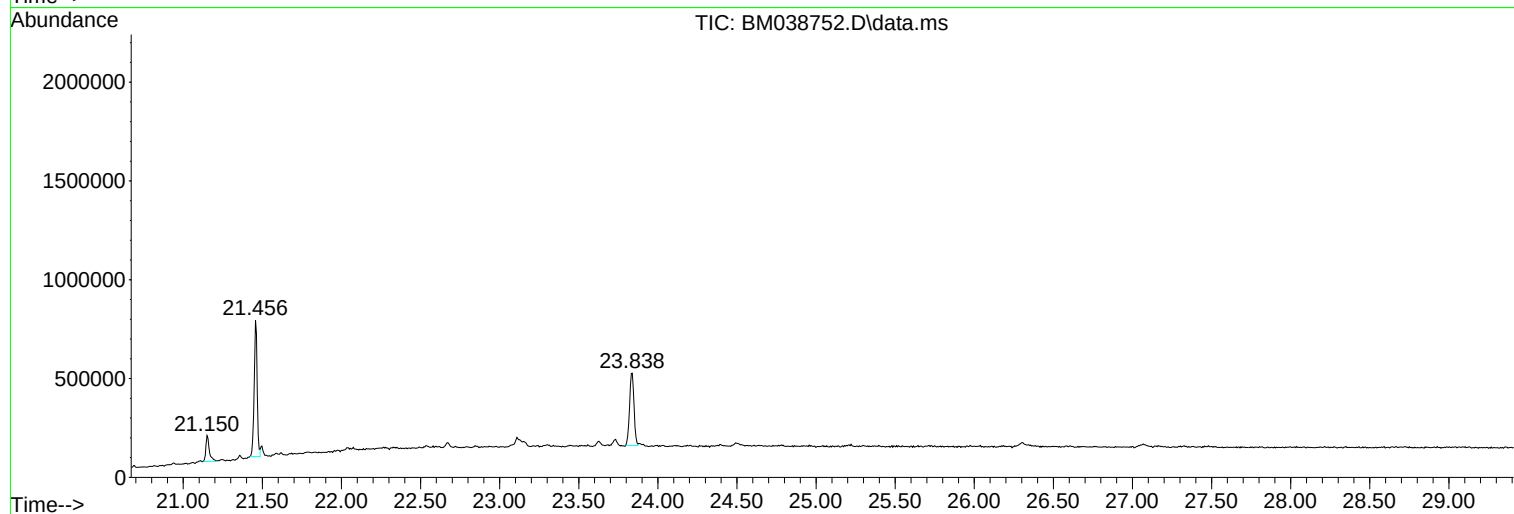
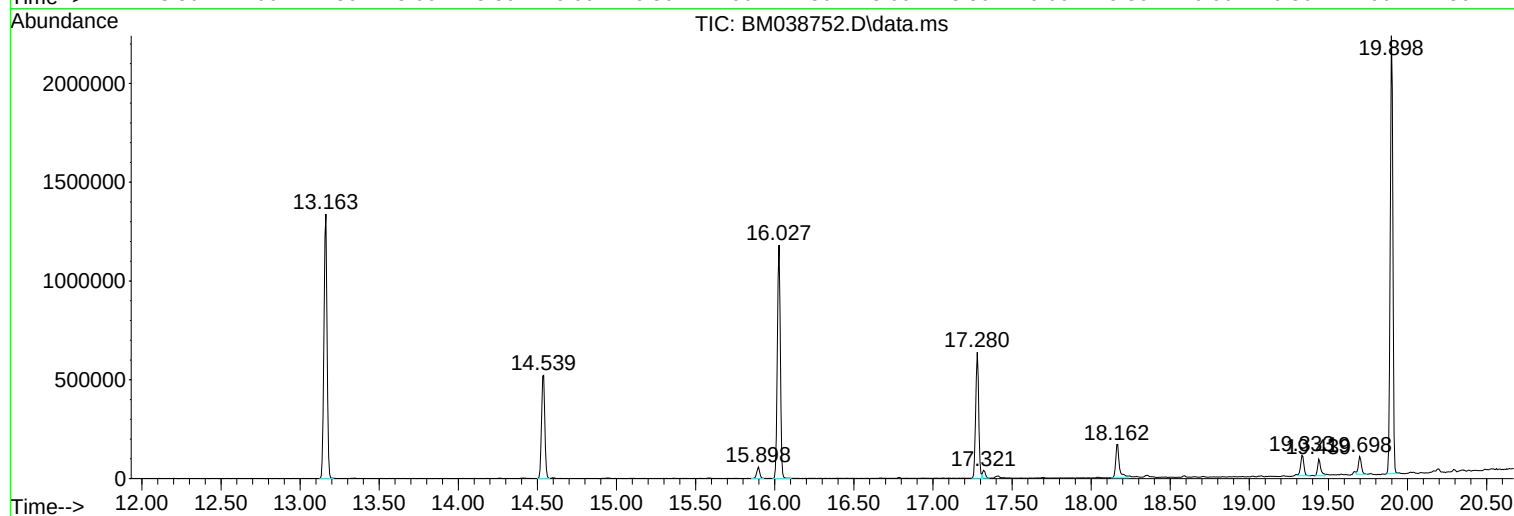
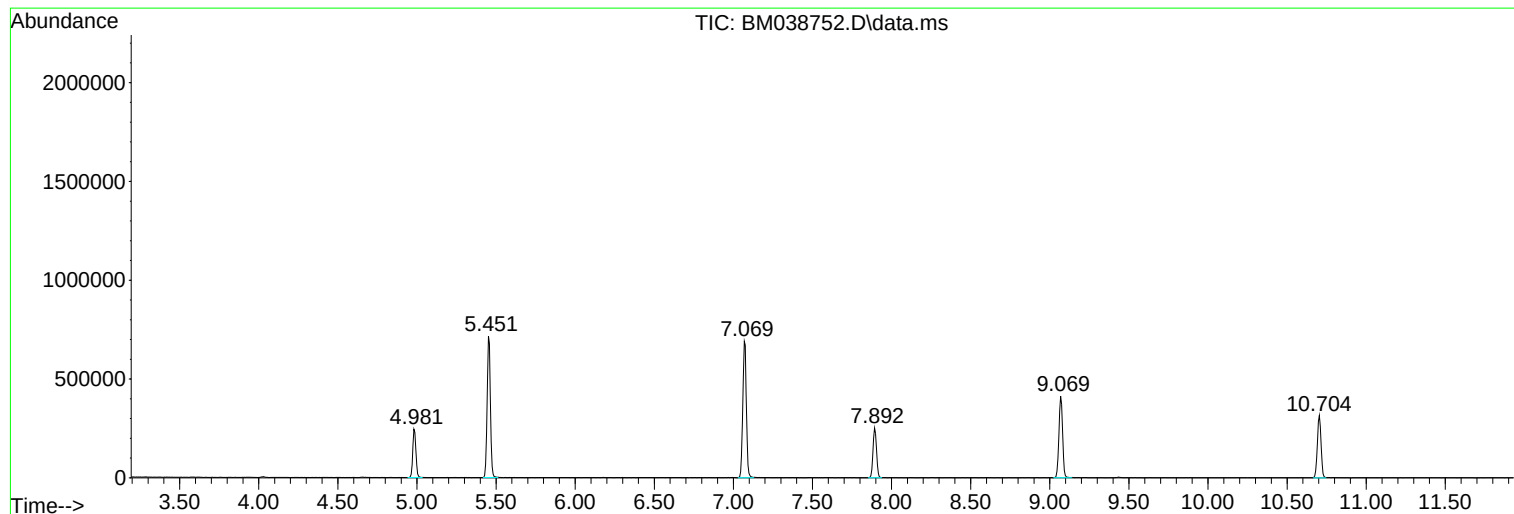
Sum of corrected areas: 14147706

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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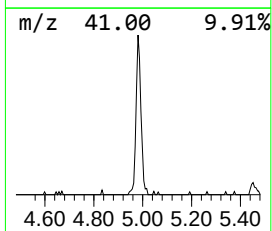
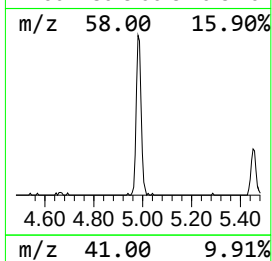
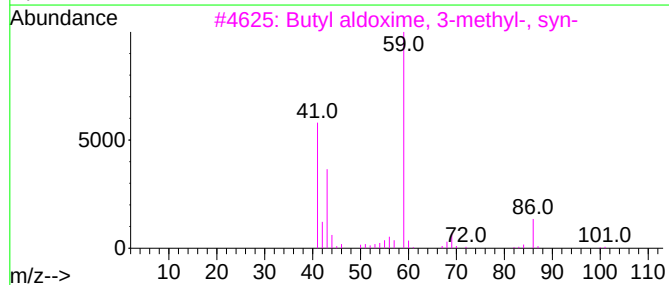
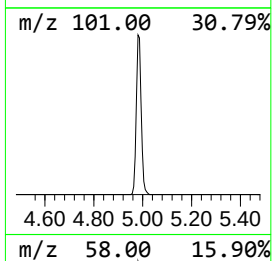
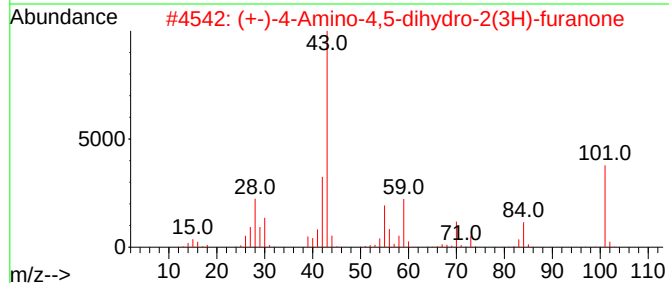
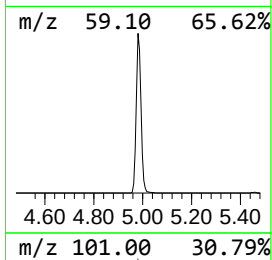
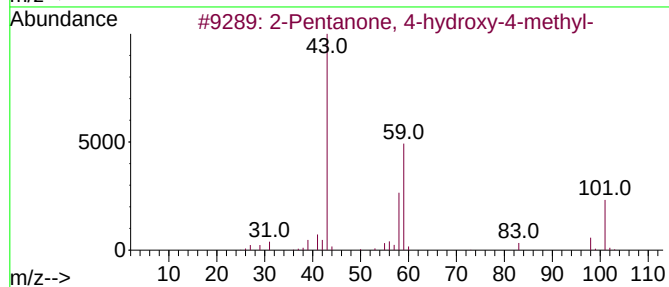
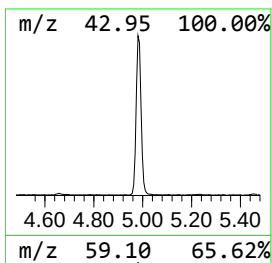
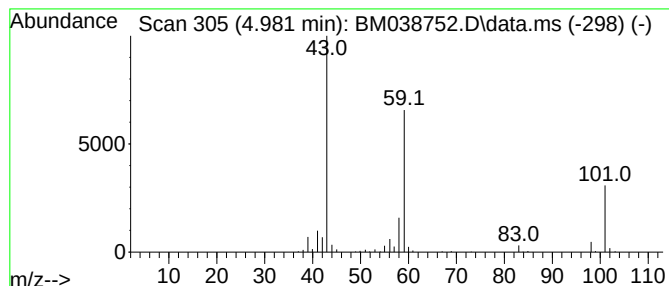
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM020123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.981	17.82 ng	337952	1,4-Dichlorobenzene-d4	7.892

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	43		
3	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	25		
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17		
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		



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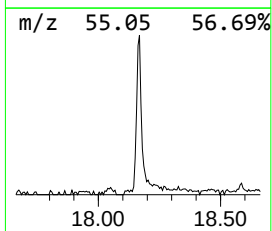
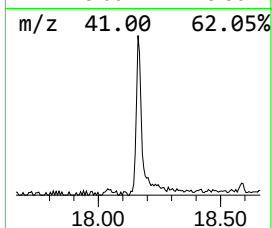
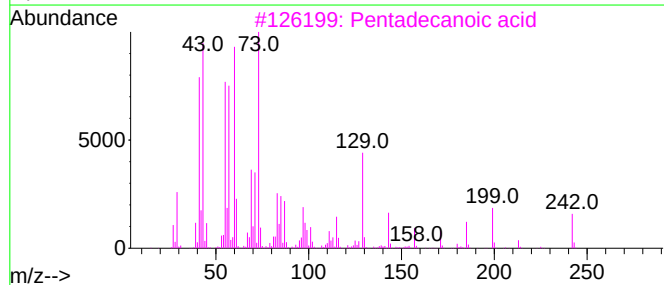
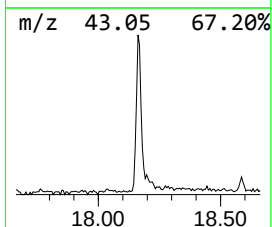
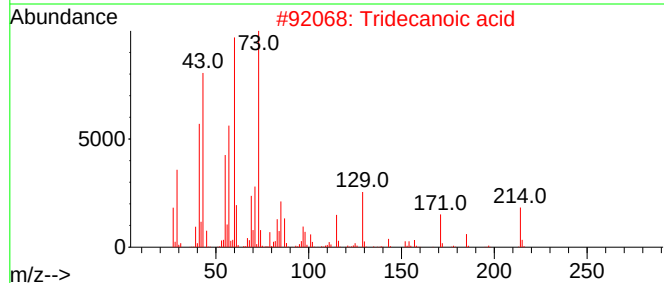
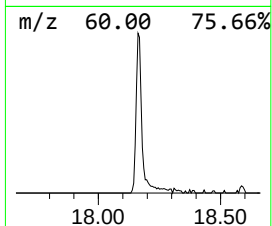
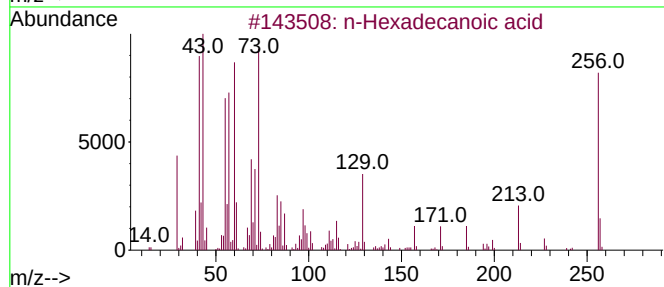
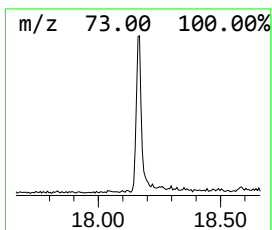
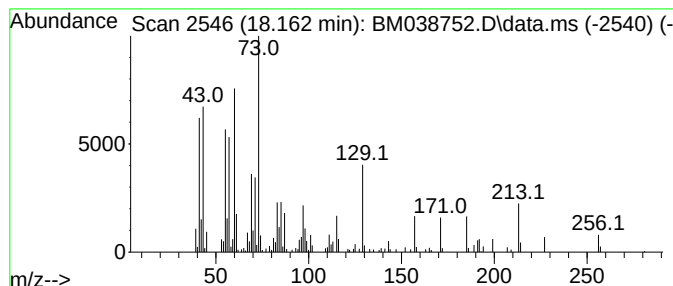
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.162	6.55 ng	279505	Phenanthrene-d10	17.280

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2			Tridecanoic acid	214	C13H26O2	000638-53-9	95
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	76
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5			n-Decanoic acid	172	C10H20O2	000334-48-5	53



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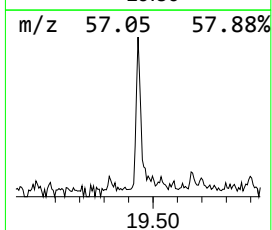
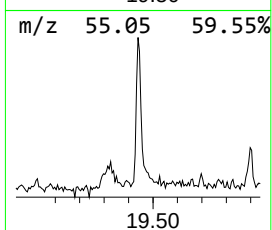
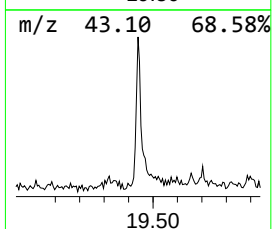
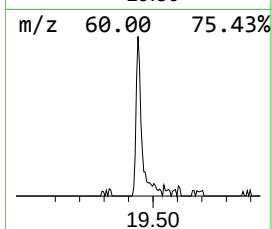
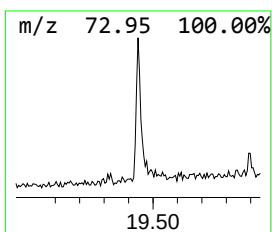
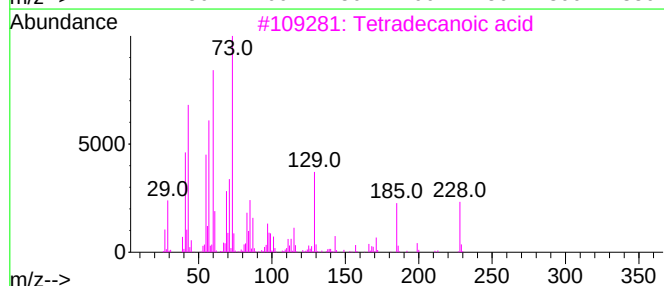
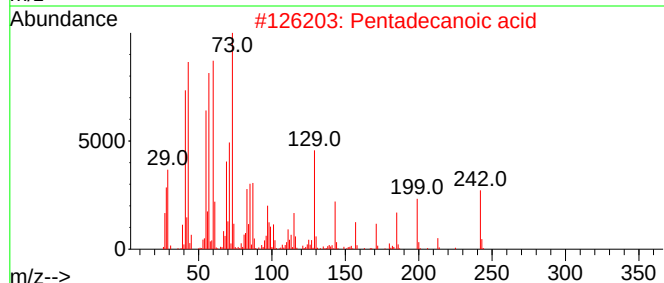
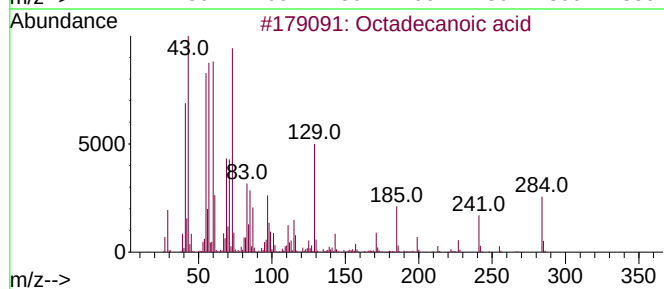
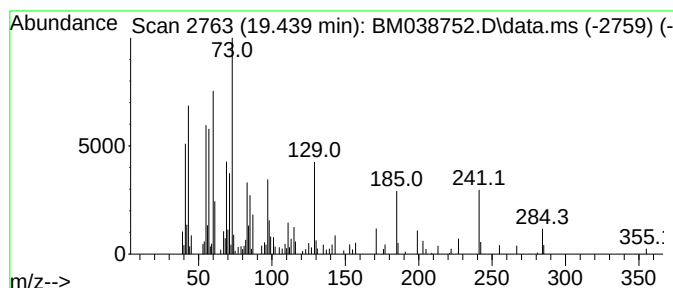
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Peak Number 3 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.439	2.60 ng	119193	Chrysene-d12	21.456

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	76
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	62
5			n-Decanoic acid	172	C10H20O2	000334-48-5	47



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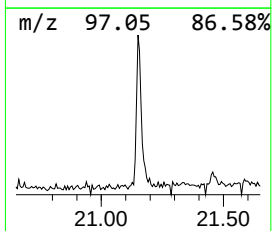
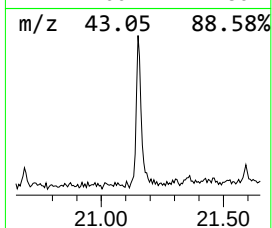
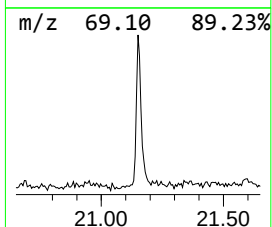
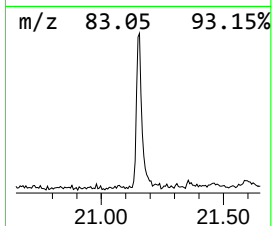
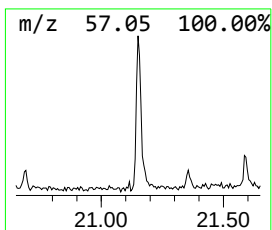
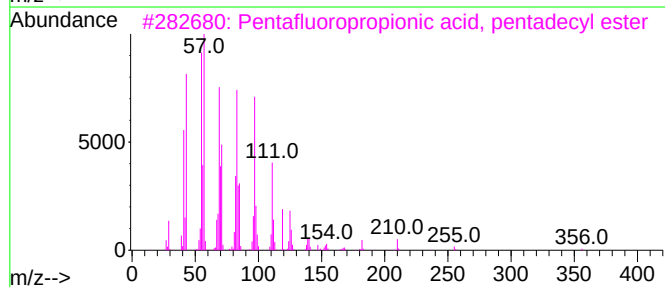
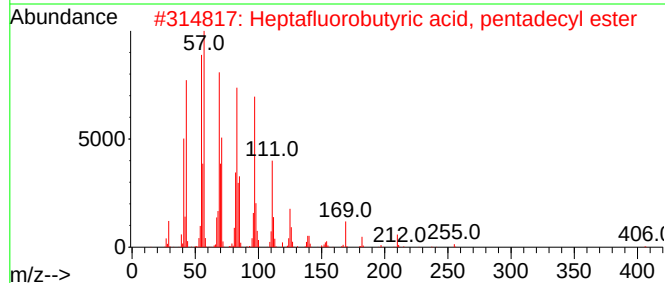
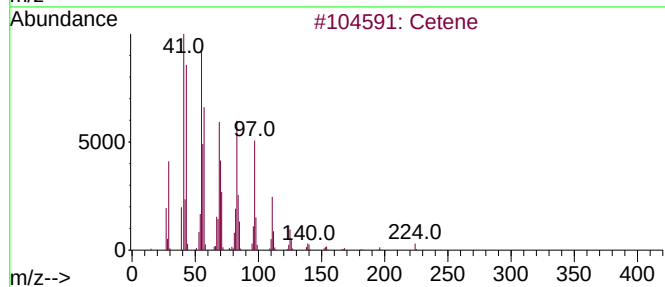
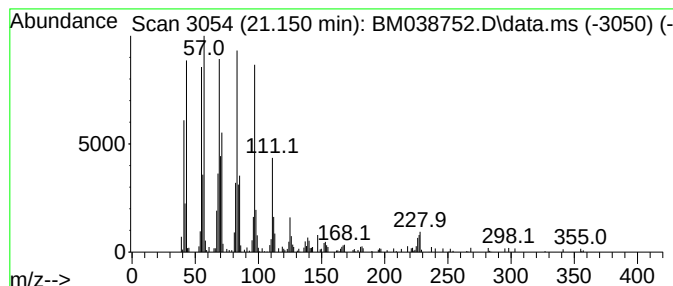
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Peak Number 4 Cetene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.150	4.35 ng	199112	Chrysene-d12	21.456

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cetene	224	C16H32	000629-73-2	94
2			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
3			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
4			Pentacos-1-ene	350	C25H50	016980-85-1	94
5			1-Hexacosene	364	C26H52	018835-33-1	94



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.981	17.8	ng	337952	1	7.892	379255	20.0
n-Hexadecanoic ...	18.162	6.5	ng	279505	4	17.280	852875	20.0
Octadecanoic acid	19.439	2.6	ng	119193	5	21.456	915270	20.0
Cetene	21.150	4.3	ng	199112	5	21.456	915270	20.0