

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM082919\
 Data File : BM022428.D
 Acq On : 30 Aug 2019 03:27
 Operator : HP/JU
 Sample : K4596-01
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 S403-K1-1.0-1.5-082819

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

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-BM082919.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.146	361	367	379	rBV	222514	333336	29.41%	5.005%
2	6.722	629	635	653	rBV	212854	367043	32.38%	5.511%
3	7.057	686	692	704	rBB	259110	393716	34.74%	5.912%
4	7.522	765	771	777	rBB	66002	99124	8.75%	1.488%
5	7.828	817	823	832	rBB	197349	311898	27.52%	4.683%
6	8.693	965	970	990	rBV	113845	217807	19.22%	3.271%
7	10.298	1236	1243	1256	rBB	61276	114924	10.14%	1.726%
8	12.786	1660	1666	1686	rBV	347173	522923	46.14%	7.852%
9	13.669	1811	1816	1823	rBB	15100	21494	1.90%	0.323%
10	14.116	1888	1892	1897	rBB2	47862	59442	5.24%	0.893%
11	14.186	1897	1904	1910	rBV	101597	150258	13.26%	2.256%
12	15.698	2155	2161	2173	rVB	344635	494242	43.61%	7.421%
13	16.951	2369	2374	2379	rBV2	130034	191317	16.88%	2.873%
14	16.998	2379	2382	2389	rVB	26490	34539	3.05%	0.519%
15	17.845	2521	2526	2530	rBV3	51297	67064	5.92%	1.007%
16	19.021	2722	2726	2738	rVB	124334	175364	15.47%	2.633%
17	19.139	2742	2746	2754	rBV3	20617	27457	2.42%	0.412%
18	19.362	2780	2784	2785	rBV	13392	14756	1.30%	0.222%
19	19.392	2785	2789	2796	rVB	87050	110148	9.72%	1.654%
20	19.598	2818	2824	2830	rBV	992338	1133435	100.00%	17.019%
21	19.904	2872	2876	2880	rVB3	10229	14935	1.32%	0.224%
22	20.198	2921	2926	2930	rBV5	5073	11988	1.06%	0.180%
23	20.298	2940	2943	2950	rVB2	19406	22124	1.95%	0.332%
24	20.727	3011	3016	3022	rBV	403787	470039	41.47%	7.058%
25	20.809	3028	3030	3033	rVB	11723	12474	1.10%	0.187%
26	20.862	3034	3039	3042	rBV5	36474	58949	5.20%	0.885%
27	21.168	3084	3091	3095	rBV2	289756	464445	40.98%	6.974%
28	21.203	3095	3097	3103	rVB	68183	77348	6.82%	1.161%
29	21.315	3114	3116	3120	rBV3	15125	14361	1.27%	0.216%
30	22.703	3347	3352	3357	rBV	109967	214301	18.91%	3.218%
31	23.262	3443	3447	3452	rVB2	55475	91645	8.09%	1.376%
32	23.350	3457	3462	3468	rBV	209742	366776	32.36%	5.507%

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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

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

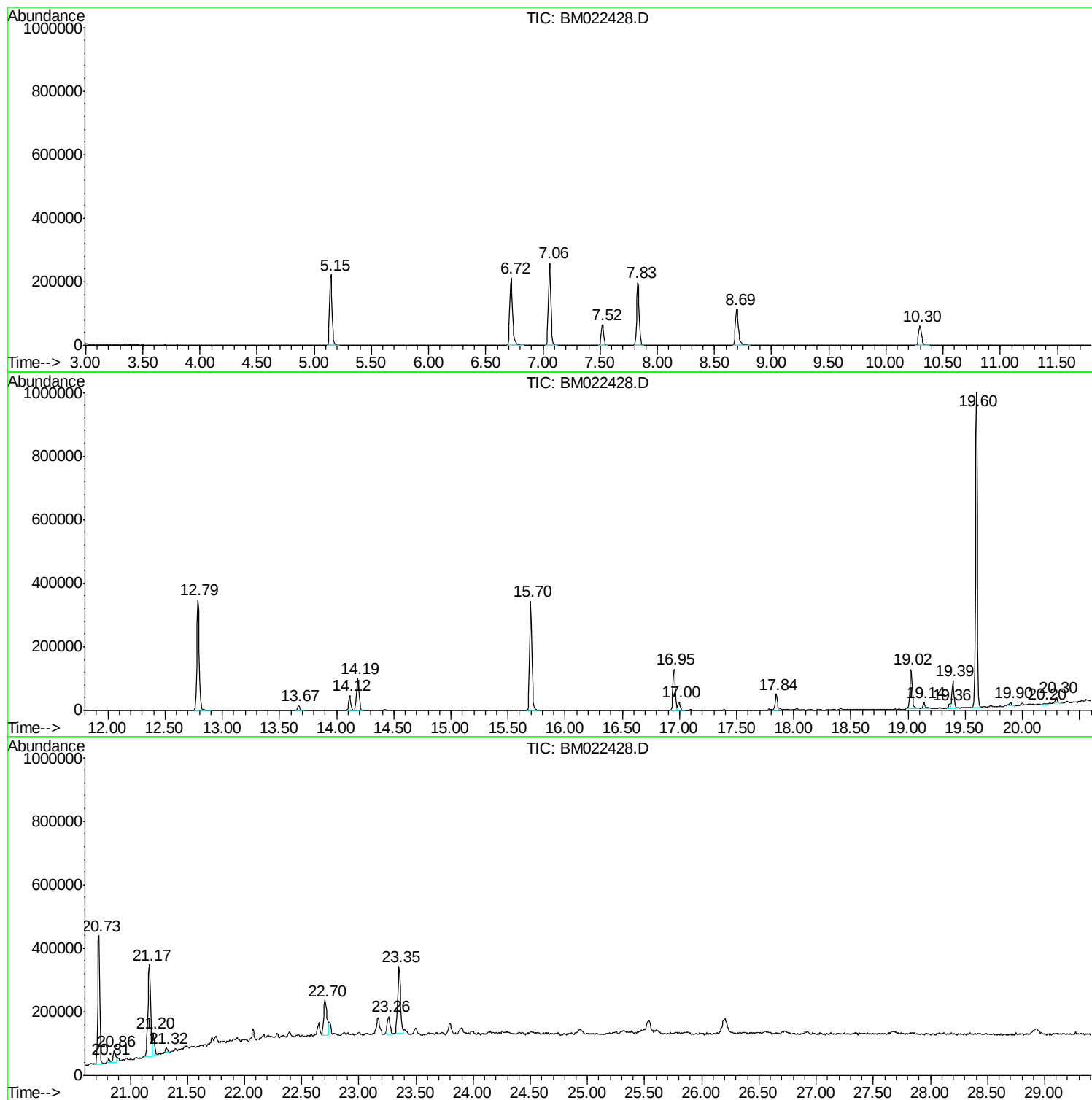
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM082919.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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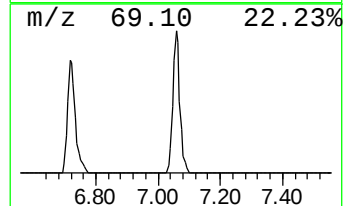
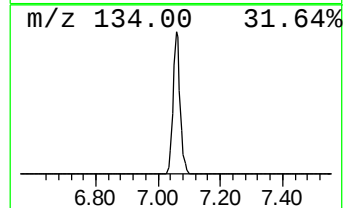
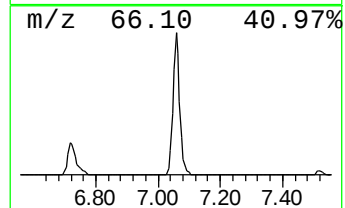
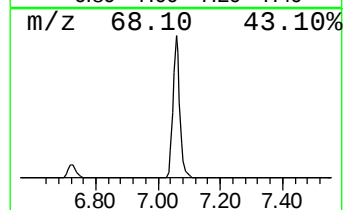
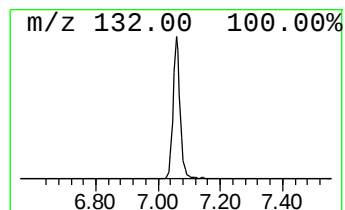
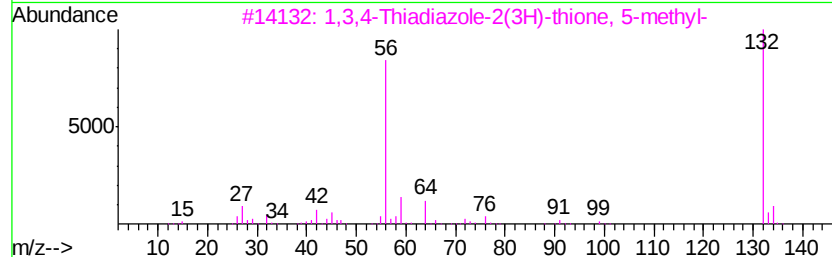
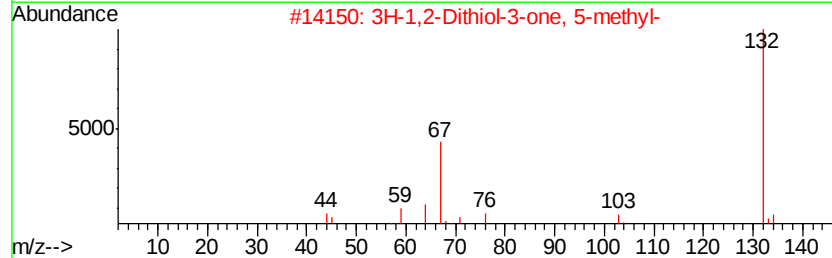
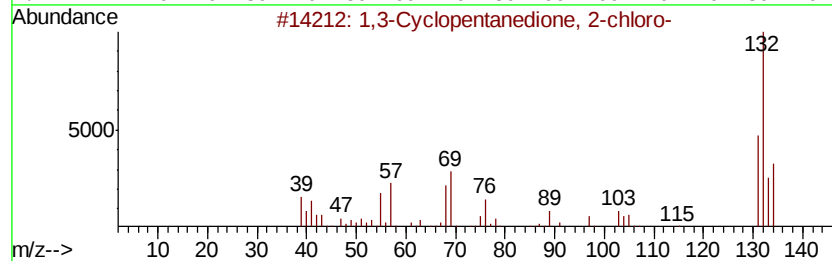
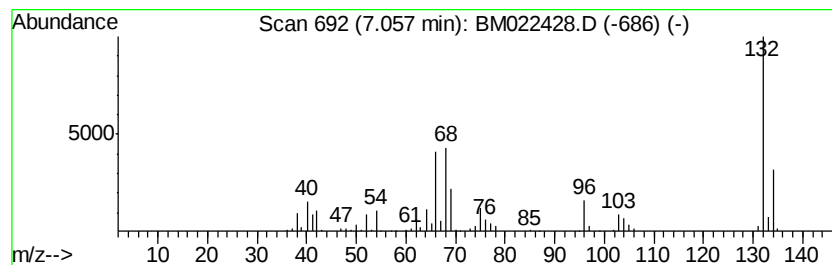
Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM082919.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown7.06 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.06	79.44 ng	393716	1,4-Dichlorobenzene-d4	7.52

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	22
2		3H-1,2-Dithiol-3-one, 5-methyl-	132	C4H4OS2	003620-08-4	14
3		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	14
4		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	14
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	14



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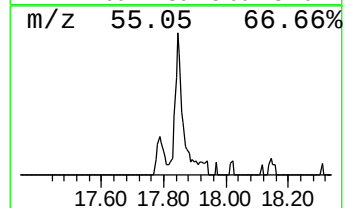
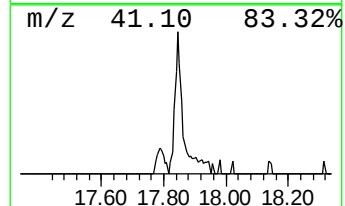
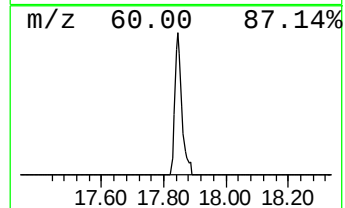
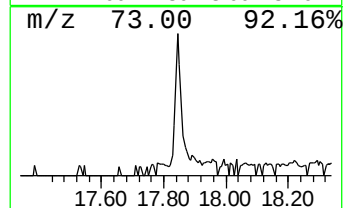
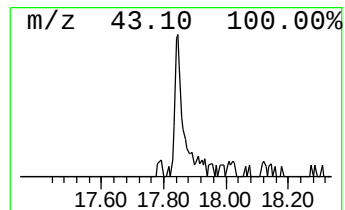
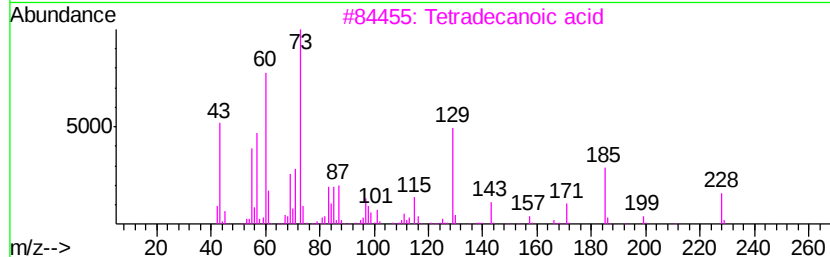
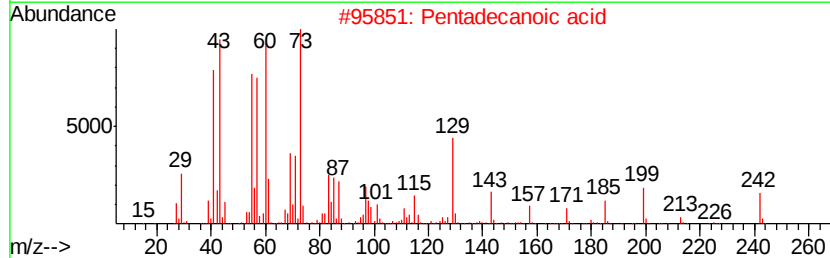
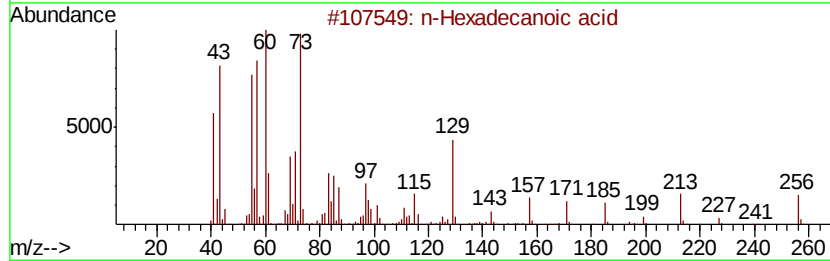
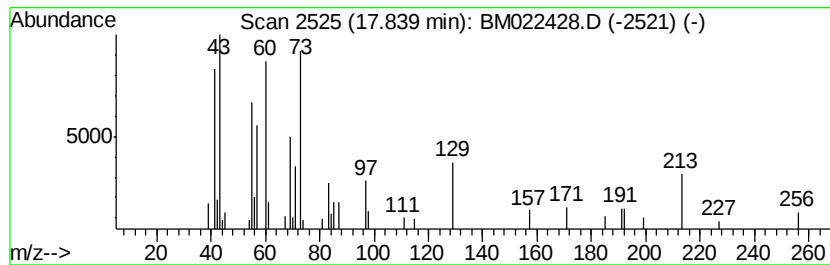
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.84	7.01 ng	67064	Phenanthrene-d10	16.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	86
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	62
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	52
4	n-Decanoic acid	172	C10H20O2	000334-48-5	43
5	Undecanoic acid, 10-bromo-	264	C11H21BrO2	018294-93-4	38



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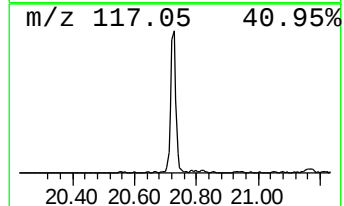
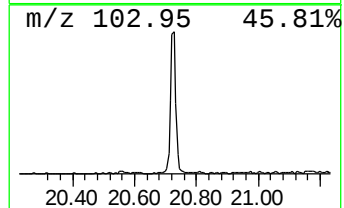
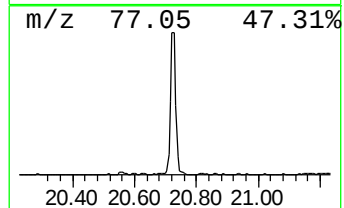
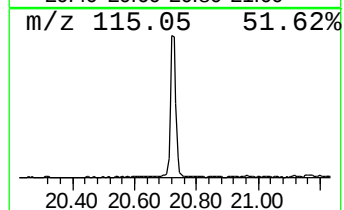
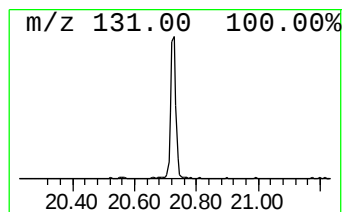
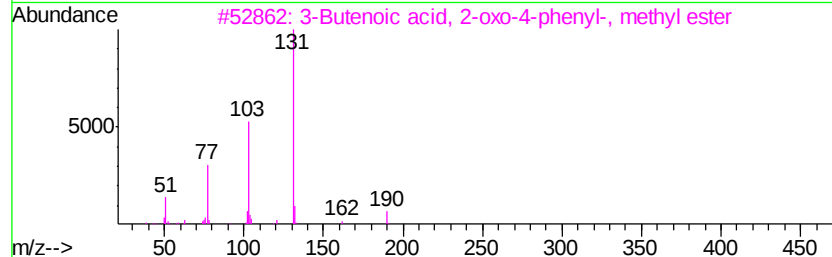
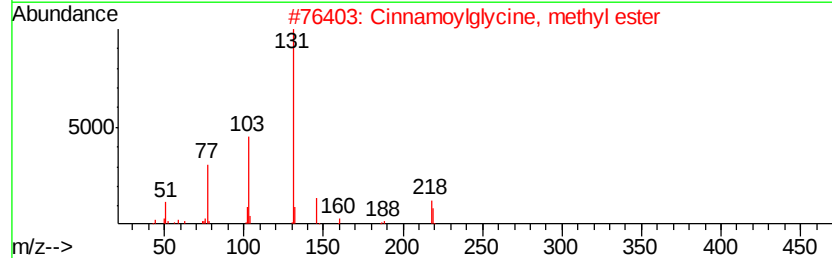
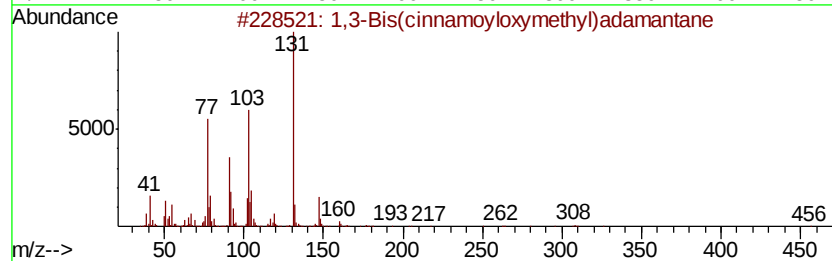
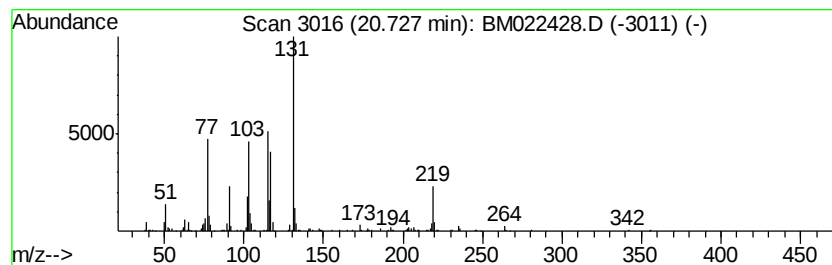
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Peak Number 5 unknown20.73 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.73	20.24 ng	470039	Chrysene-d12	21.17

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Bis(cinnamoyloxymethyl)adama...	456	C30H32O4	303797-58-2	47
2		Cinnamoylglycine, methyl ester	219	C12H13NO3	040778-04-9	43
3		3-Butenoic acid, 2-oxo-4-phenyl-...	190	C11H10O3	1000142-22-4	43
4		1-(2-Vinylphenyl)propan-1-one	160	C11H12O	052095-41-7	43
5		4-Methylcoumarine-7-cinnamate	306	C19H14O4	300829-05-4	43



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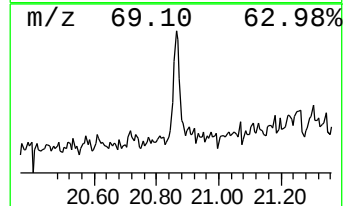
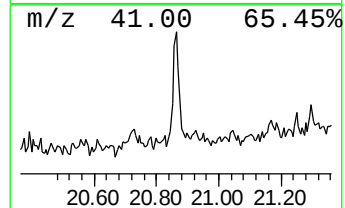
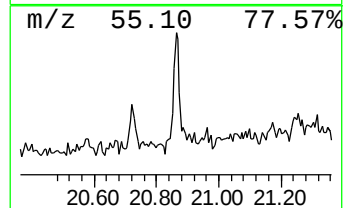
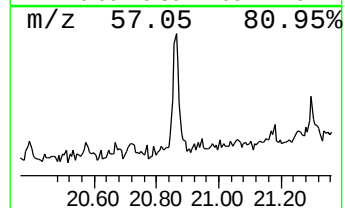
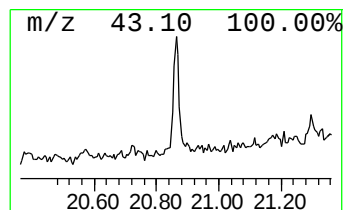
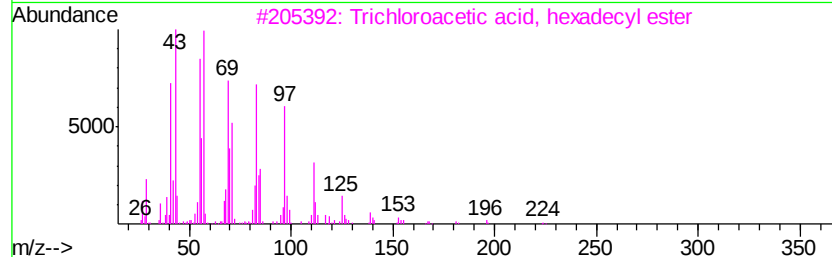
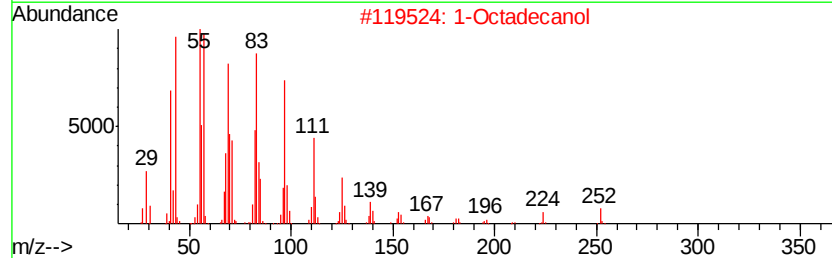
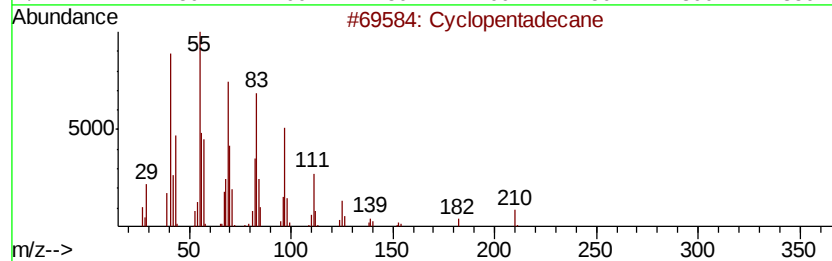
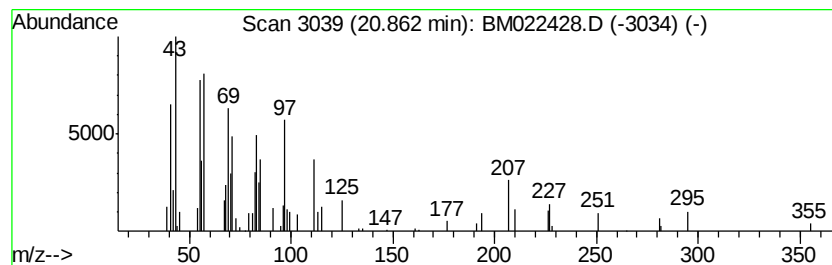
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Cyclopentadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.86	2.54 ng	58949	Chrysene-d12	21.17
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Cyclopentadecane	210 C15H30	000295-48-7 96
2		1-Octadecanol	270 C18H38O	000112-92-5 64
3		Trichloroacetic acid, hexadecyl ...	386 C18H33Cl3O2	074339-54-1 62
4		Heptafluorobutyric acid, n-octad...	466 C22H37F7O2	000400-57-7 58
5		Eicosyl trifluoroacetate	394 C22H41F3O2	1000351-75-2 58



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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown7.06	7.06	79.4	ng	393716	1	7.52	99124	20.0
1,6-Cyclodecadien...	14.12	7.9	ng	59442	3	14.19	150258	20.0
n-Hexadecanoic acid	17.84	7.0	ng	67064	4	16.95	191317	20.0
unknown20.73	20.73	20.2	ng	470039	5	21.17	464445	20.0
Cyclopentadecane	20.86	2.5	ng	58949	5	21.17	464445	20.0