

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG031921\
 Data File : BG048437.D
 Acq On : 19 Mar 2021 23:49
 Operator : CG/JU
 Sample : M1721-03 2X
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 TR-08-031821

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_G\METHODS\8270-BG031821.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG048437.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.183	310	314	320	rBV4	9266	15721	1.14%	0.131%
2	5.653	387	394	403	rBV	360747	582721	42.26%	4.873%
3	7.251	658	666	676	rBV	382226	678312	49.19%	5.673%
4	8.109	802	812	822	rBV	237242	393066	28.50%	3.287%
5	9.272	998	1010	1017	rBV	247733	428737	31.09%	3.585%
6	10.929	1284	1292	1301	rBV	291827	522200	37.87%	4.367%
7	13.367	1701	1707	1716	rVB	589695	915215	66.37%	7.654%
8	14.190	1841	1847	1851	rBV2	26418	46865	3.40%	0.392%
9	14.584	1911	1914	1919	rVB4	10030	15056	1.09%	0.126%
10	14.748	1933	1942	1950	rBV	525170	809150	58.68%	6.767%
11	15.142	2005	2009	2013	rVB4	13494	19722	1.43%	0.165%
12	15.359	2044	2046	2051	rBV5	8085	14164	1.03%	0.118%
13	16.235	2187	2195	2201	rBV	636208	944542	68.50%	7.899%
14	16.475	2229	2236	2242	rVB10	14272	30641	2.22%	0.256%
15	16.728	2274	2279	2283	rBV6	7920	14023	1.02%	0.117%
16	17.498	2404	2410	2415	rBV	698453	1037664	75.25%	8.678%
17	17.539	2415	2417	2423	rVB	42885	57849	4.20%	0.484%
18	17.985	2490	2493	2497	rVB6	9500	14318	1.04%	0.120%
19	18.162	2518	2523	2527	rBV	73151	82787	6.00%	0.692%
20	18.379	2556	2560	2566	rBV2	84708	124093	9.00%	1.038%
21	18.420	2566	2567	2572	rVB5	15823	19874	1.44%	0.166%
22	18.555	2586	2590	2592	rBV5	14830	18445	1.34%	0.154%
23	19.149	2688	2691	2697	rVB2	54769	69749	5.06%	0.583%
24	19.296	2711	2716	2719	rVV	385022	488240	35.41%	4.083%
25	19.325	2719	2721	2729	rVB3	291499	380752	27.61%	3.184%
26	19.460	2740	2744	2747	rBV	33729	38989	2.83%	0.326%
27	19.548	2754	2759	2764	rBV	154709	217457	15.77%	1.819%
28	19.642	2773	2775	2778	rVB4	20603	20478	1.49%	0.171%
29	19.877	2812	2815	2817	rBV4	29663	36891	2.68%	0.309%
30	19.913	2817	2821	2826	rVB	115952	170782	12.38%	1.428%
31	20.107	2849	2854	2859	rBV	1122330	1378989	100.00%	11.532%
32	20.253	2876	2879	2885	rVB6	32585	46671	3.38%	0.390%
33	21.417	3074	3077	3083	rBV4	59589	88015	6.38%	0.736%
34	21.793	3133	3141	3147	rBV	681054	1200044	87.02%	10.036%
35	25.130	3701	3709	3720	rVB2	364520	1035521	75.09%	8.660%

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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_G\METHODS\8270-BG031821.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

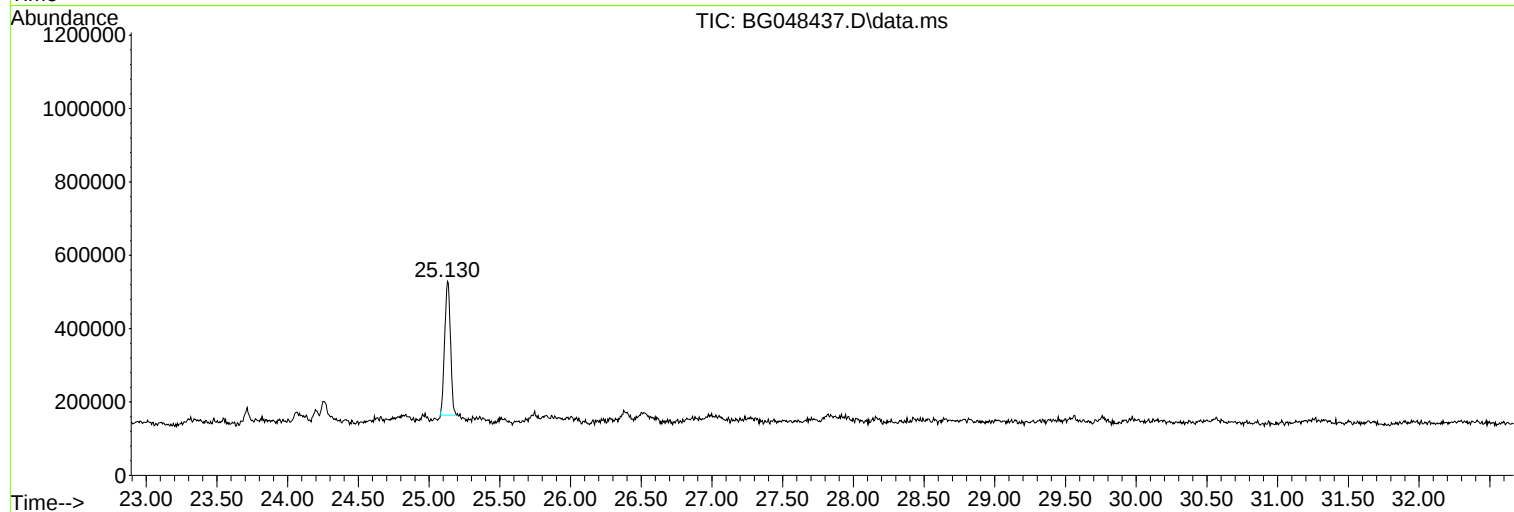
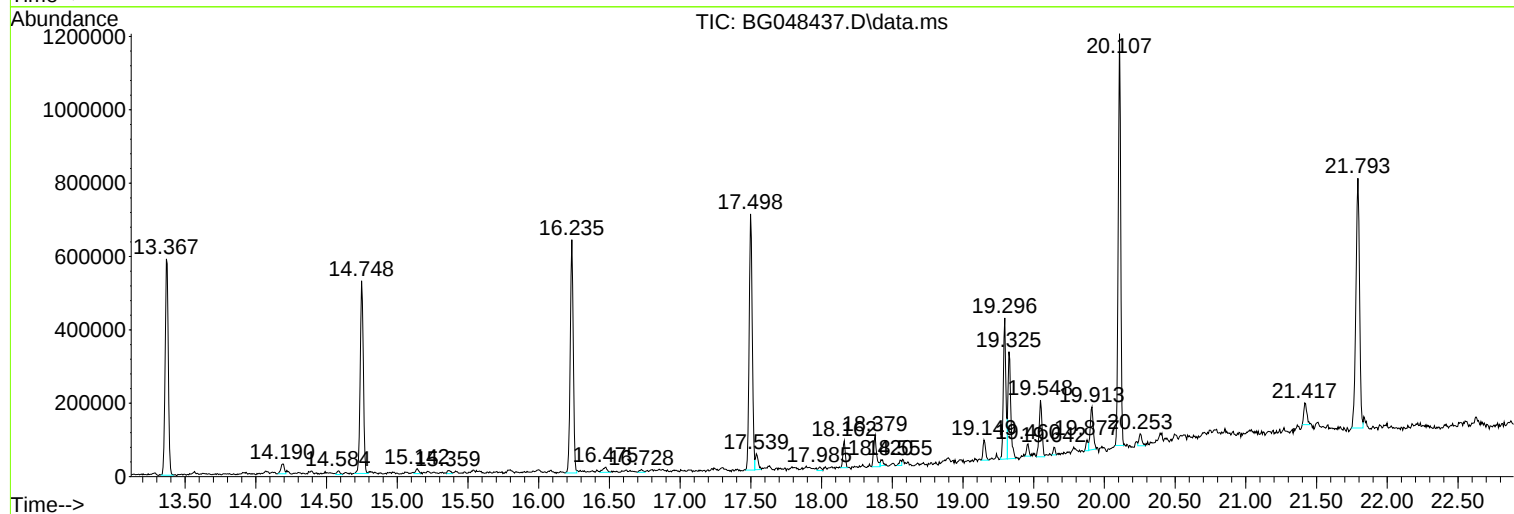
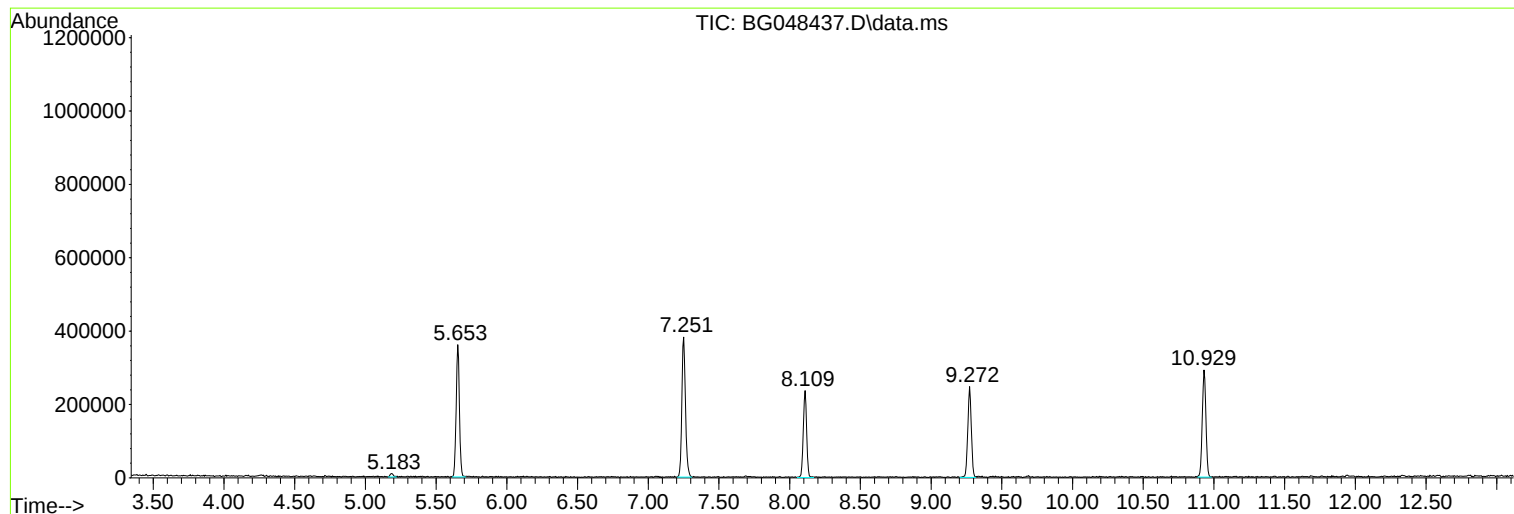
Sum of corrected areas: 11957743

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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG031821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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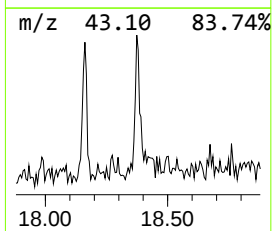
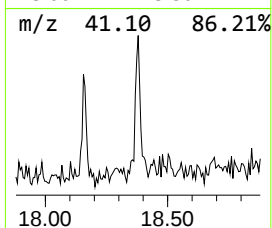
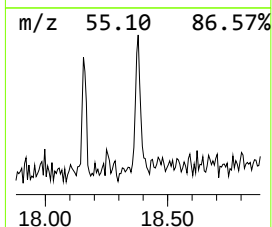
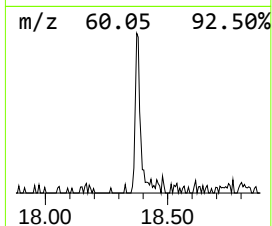
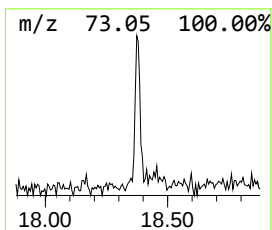
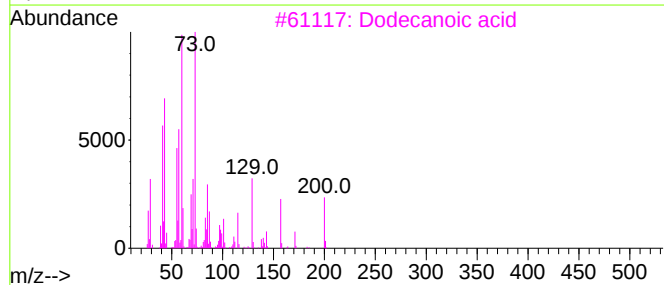
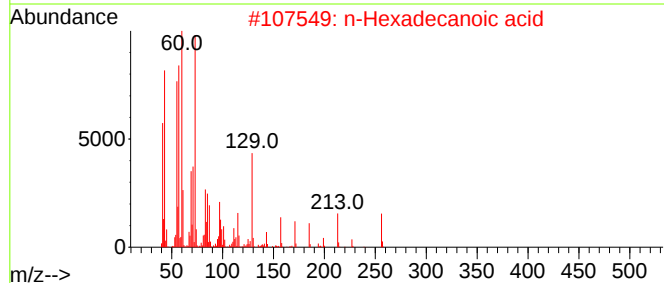
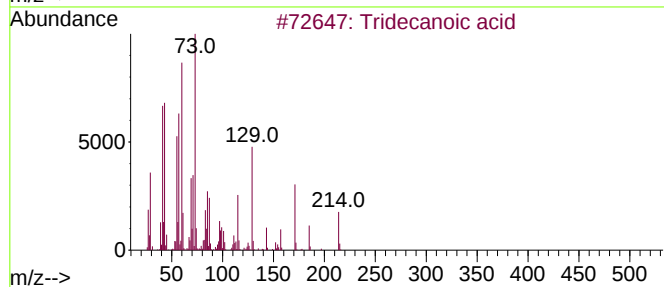
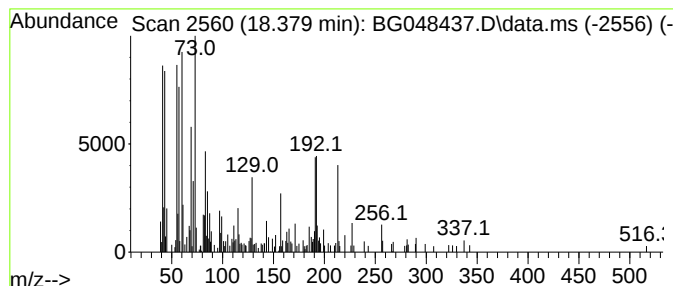
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG031821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Tridecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.379	2.39 ng	124093	Phenanthrene-d10	17.498

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecanoic acid	214	C13H26O2	000638-53-9	90
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	70
3			Dodecanoic acid	200	C12H24O2	000143-07-7	45
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	27
5			Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NO5	029926-41-8	22



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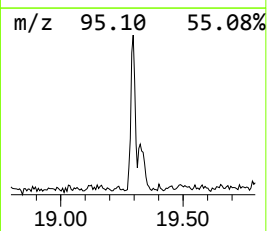
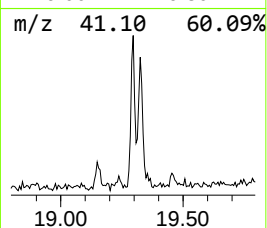
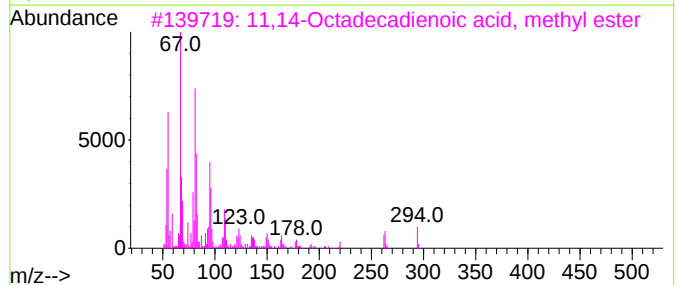
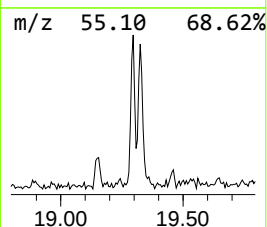
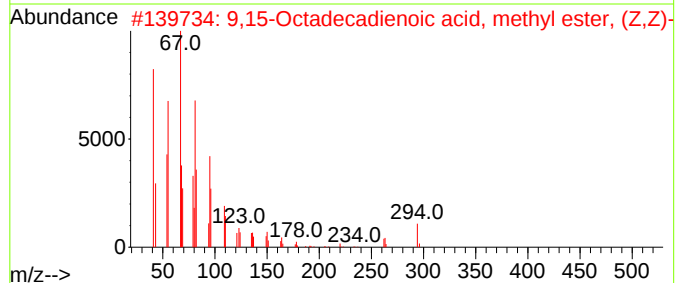
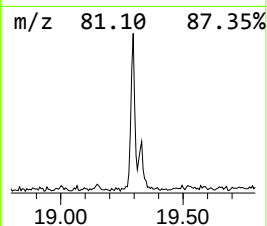
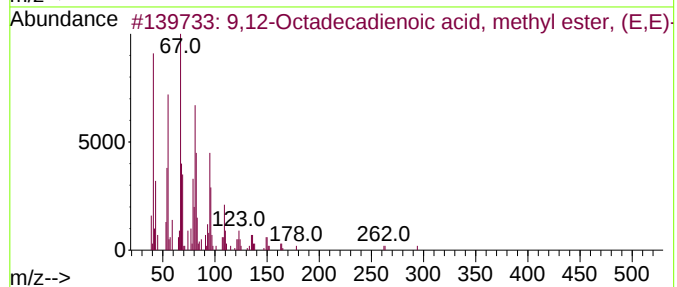
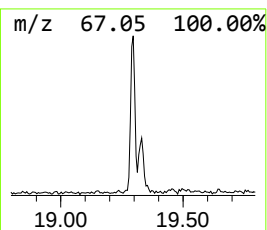
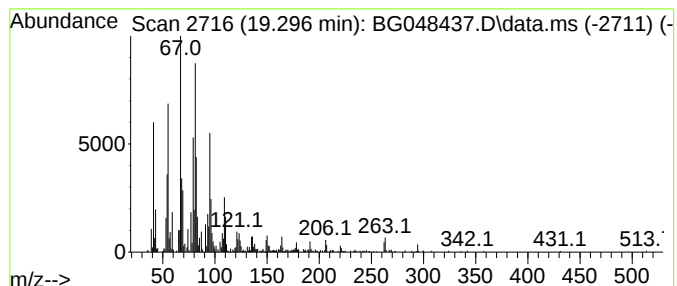
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Peak Number 2 9,12-Octadecadienoic acid, ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.296	9.41 ng	488240	Phenanthrene-d10	17.498	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	98
2	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	93
3	11,14-Octadecadienoic acid, meth...	294	C19H34O2	056554-61-1	91
4	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	89
5	8-Hexadecyne	222	C16H30	019781-86-3	81



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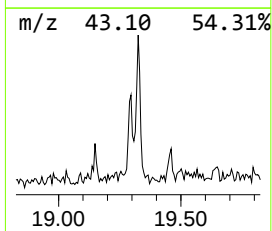
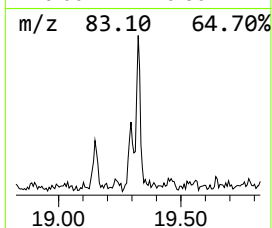
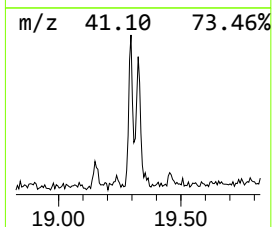
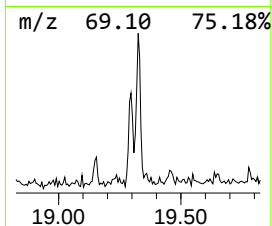
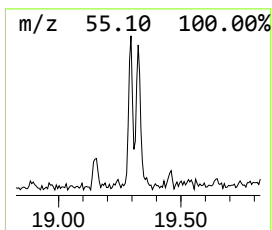
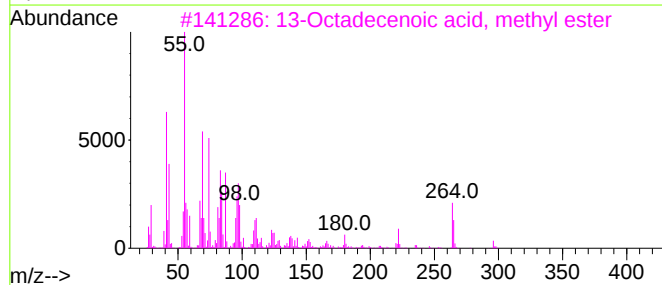
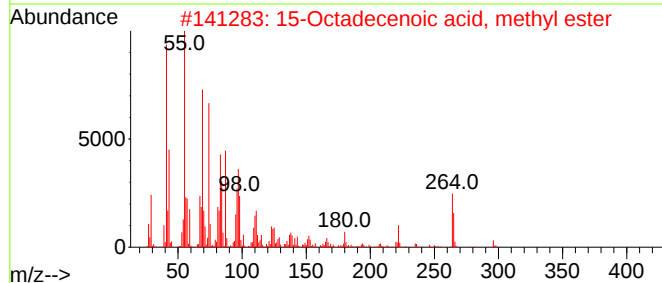
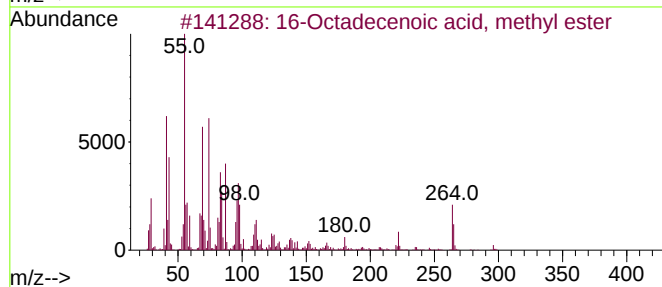
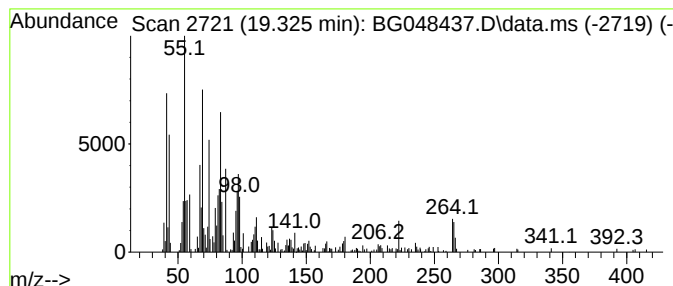
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TIC Library : C:\Database\NIST11.L
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Peak Number 3 16-Octadecenoic acid, methyl... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.325	7.34 ng	380752	Phenanthrene-d10	17.498

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	95
2			15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	92
3			13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	92
4			9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	92
5			5-Octadecenoic acid, methyl ester	296	C19H36O2	056554-45-1	80



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Tridecanoic acid	18.379	2.4	ng	124093	4	17.498	1037660	20.0
9,12-Octadecadi...	19.296	9.4	ng	488240	4	17.498	1037660	20.0
16-Octadecenoic...	19.325	7.3	ng	380752	4	17.498	1037660	20.0