

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM031521\
 Data File : BM029141.D
 Acq On : 15 Mar 2021 21:51
 Operator : CG/JU
 Sample : M1668-01 5X
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 CL-02-031221

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-BM022321.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM029141.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.205	373	377	386	rBB	25175	35712	4.40%	1.497%
2	6.834	649	654	663	rBB2	24779	38443	4.74%	1.611%
3	7.610	781	786	793	rBB	36090	53421	6.58%	2.239%
4	8.787	981	986	994	rBB	15000	23909	2.95%	1.002%
5	10.404	1255	1261	1267	rBV	45806	73242	9.02%	3.070%
6	12.892	1679	1684	1690	rBB	36476	48276	5.95%	2.024%
7	14.286	1915	1921	1927	rBB	66101	90670	11.17%	3.800%
8	15.792	2172	2177	2182	rBB	25227	32196	3.97%	1.350%
9	17.033	2383	2388	2392	rBV	76195	103308	12.73%	4.330%
10	17.080	2392	2396	2401	rVV	33859	44124	5.44%	1.849%
11	17.169	2404	2411	2418	rBV	7248	10510	1.29%	0.441%
12	17.704	2497	2502	2507	rBV	44016	50820	6.26%	2.130%
13	17.933	2538	2541	2550	rVB3	13286	21776	2.68%	0.913%
14	18.104	2564	2570	2574	rBV2	5245	8154	1.00%	0.342%
15	18.851	2689	2697	2700	rBV	120983	146576	18.06%	6.144%
16	18.880	2700	2702	2707	rVV	141840	171986	21.19%	7.209%
17	19.016	2721	2725	2732	rVB	25838	29480	3.63%	1.236%
18	19.098	2732	2739	2746	rBV	54986	86335	10.64%	3.619%
19	19.221	2757	2760	2768	rBV5	8774	14175	1.75%	0.594%
20	19.463	2797	2801	2810	rVB	37175	53040	6.53%	2.223%
21	19.663	2831	2835	2840	rVB	67067	77268	9.52%	3.239%
22	19.968	2882	2887	2891	rVB2	10096	14883	1.83%	0.624%
23	20.468	2967	2972	2975	rBV2	9595	11487	1.42%	0.481%
24	20.980	3025	3059	3060	rBV	175002	811730	100.00%	34.024%
25	21.215	3093	3099	3103	rBV2	114339	165110	20.34%	6.921%
26	21.251	3103	3105	3111	rVB	18336	22994	2.83%	0.964%
27	21.362	3121	3124	3129	rVB2	15324	21169	2.61%	0.887%
28	23.356	3458	3463	3469	rVB	72581	124967	15.40%	5.238%

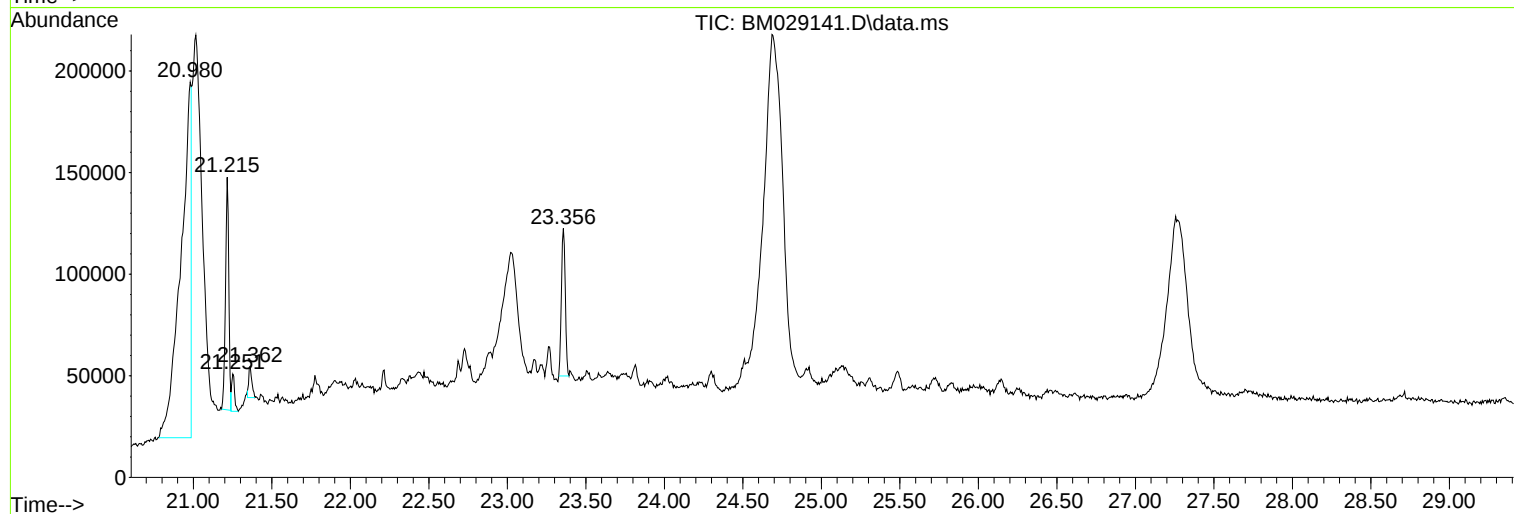
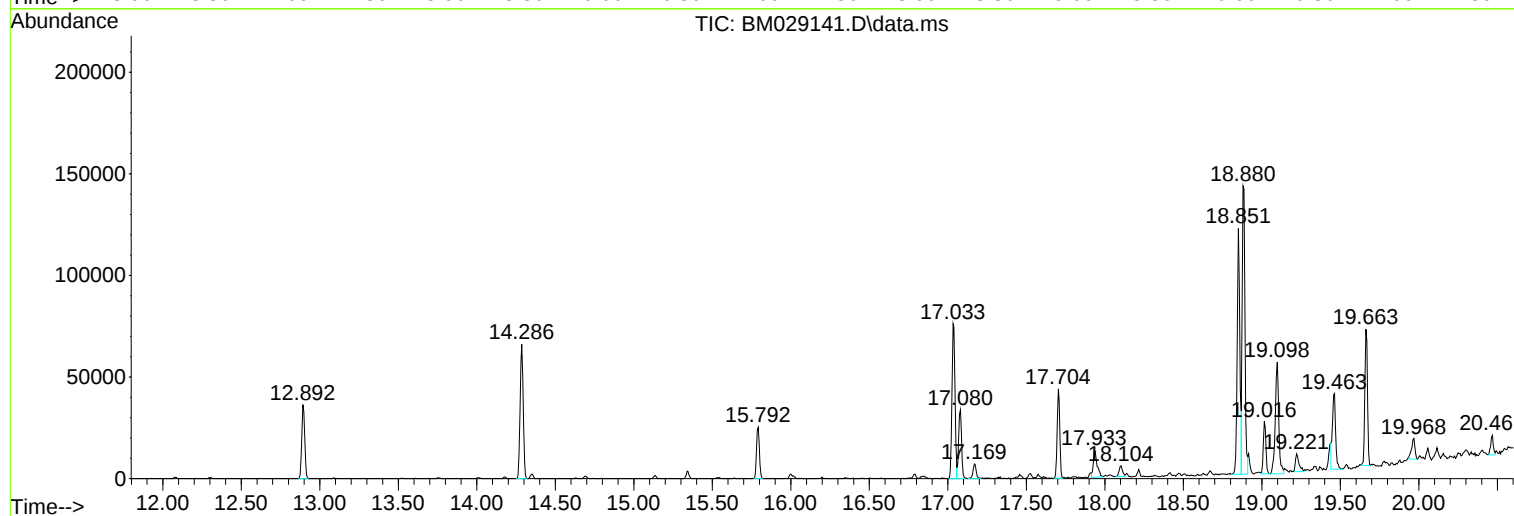
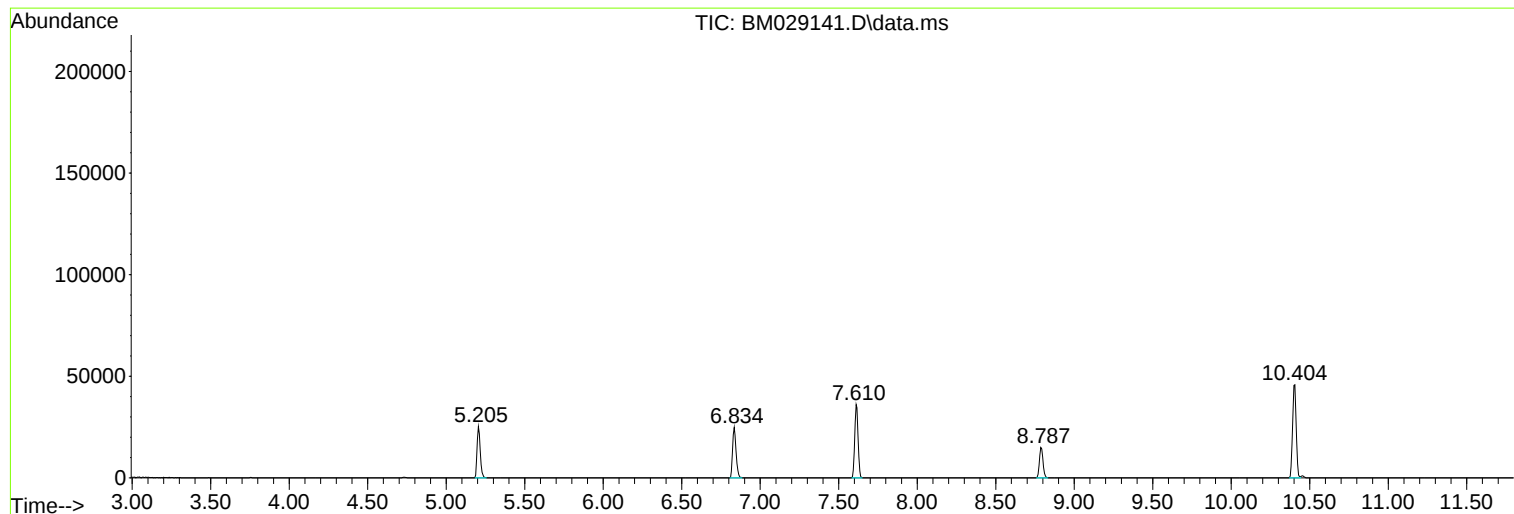
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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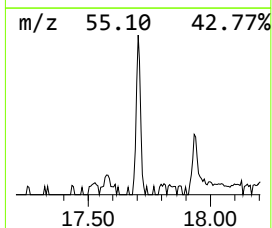
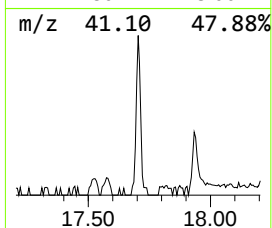
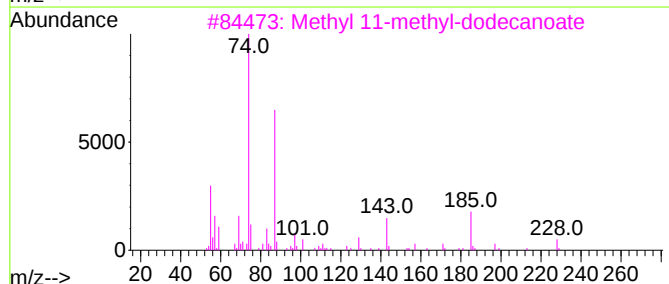
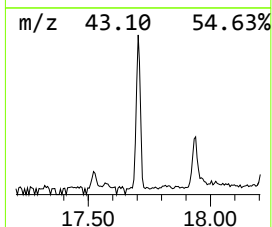
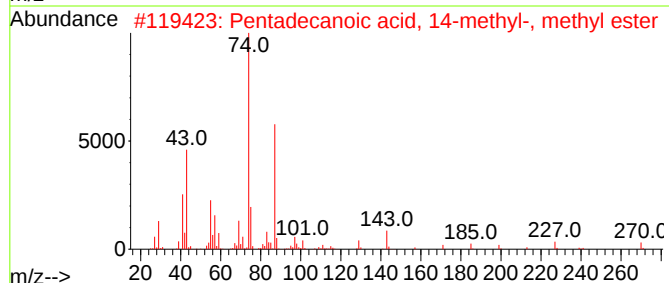
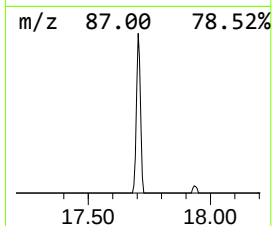
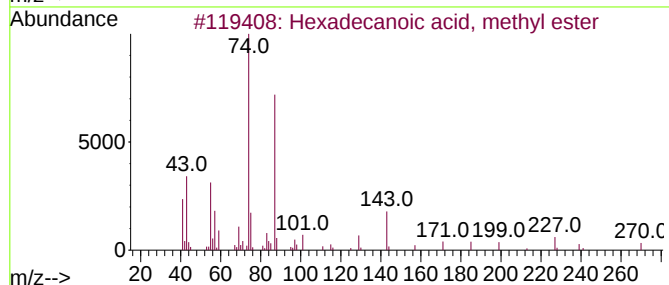
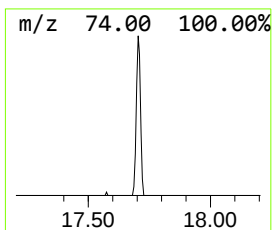
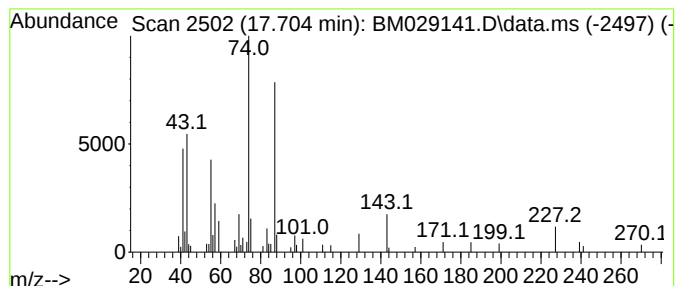
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Hexadecanoic acid, methyl e... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
17.704	9.84 ng	50820	Phenanthrene-d10	17.033	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	98
2	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	94
3	Methyl 11-methyl-dodecanoate	228	C14H28O2	1000336-45-1	83
4	Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	83
5	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	80



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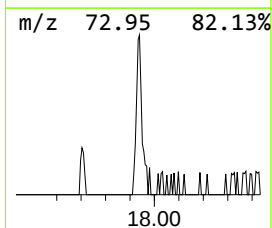
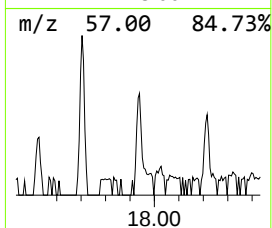
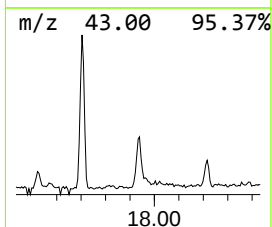
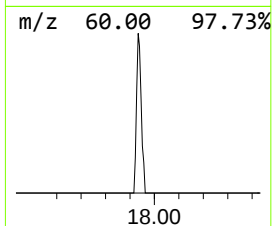
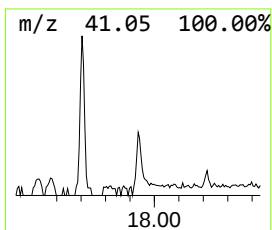
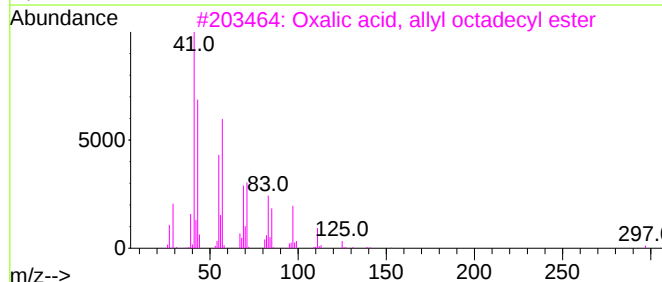
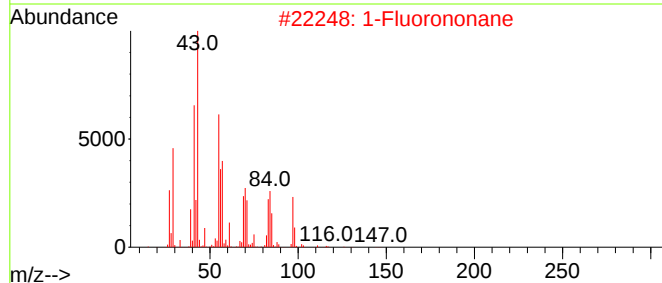
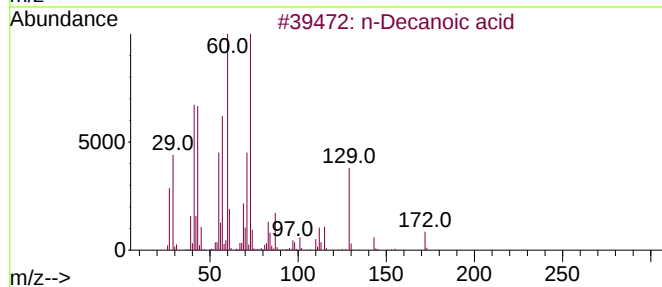
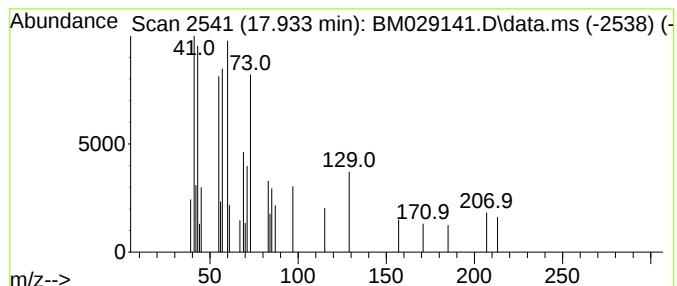
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Peak Number 2 n-Decanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.933	4.22 ng	21776	Phenanthrene-d10	17.033

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Decanoic acid	172	C10H20O2	000334-48-5	59
2			1-Fluorononane	146	C9H19F	000463-18-3	22
3			Oxalic acid, allyl octadecyl ester	382	C23H42O4	1000309-24-5	14
4			Tetratriacontyl pentafluoropropi...	641	C37H69F5O2	1000351-81-5	14
5			.beta.-D-Mannofuranoside, 1-O-(1...	332	C17H32O6	1000155-29-9	14



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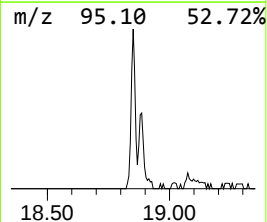
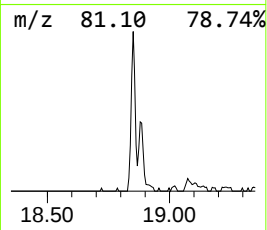
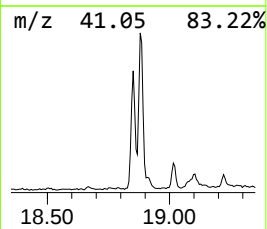
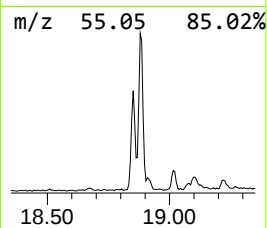
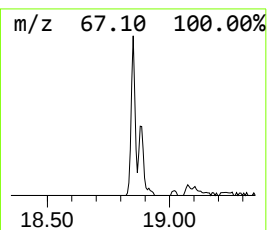
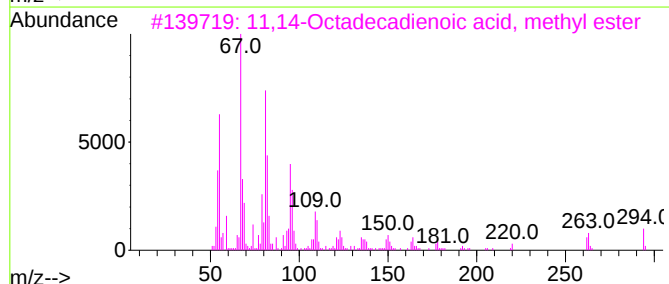
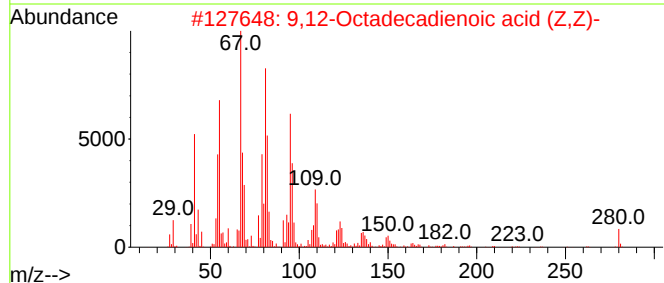
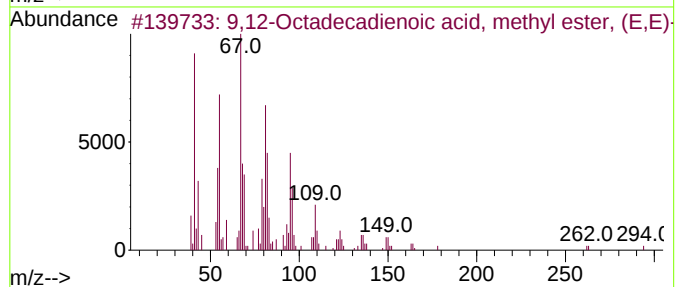
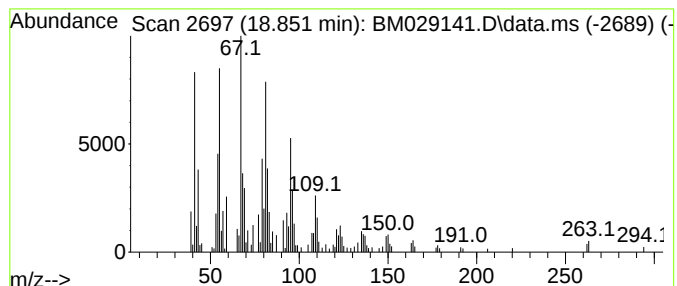
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 9,12-Octadecadienoic acid, ... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.851	28.38 ng	146576	Phenanthrene-d10	17.033
Hit#	of 5	Tentative ID	MW MolForm	CAS# Qual
1		9,12-Octadecadienoic acid, methy...	294 C19H34O2	002566-97-4 98
2		9,12-Octadecadienoic acid (Z,Z)-	280 C18H32O2	000060-33-3 94
3		11,14-Octadecadienoic acid, meth...	294 C19H34O2	056554-61-1 93
4		2-Chloroethyl linoleate	342 C20H35ClO2	025525-76-2 93
5		9,12-Octadecadienoic acid, methy...	294 C19H34O2	002462-85-3 93



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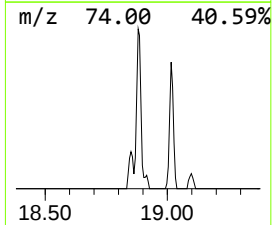
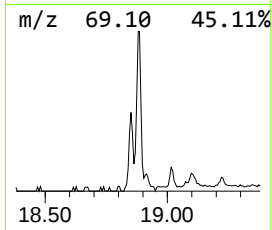
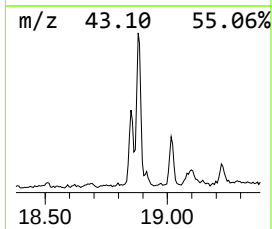
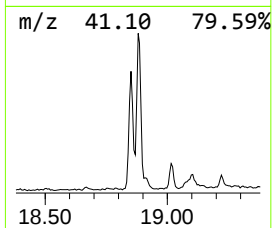
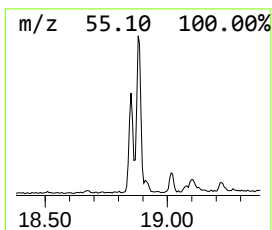
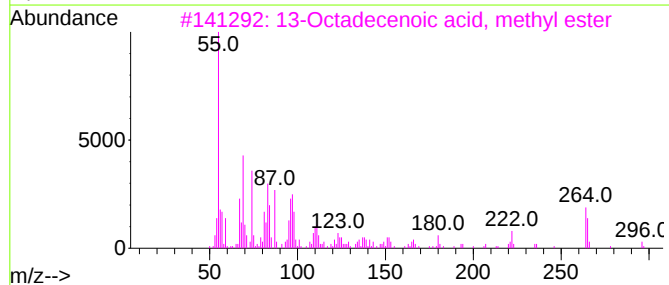
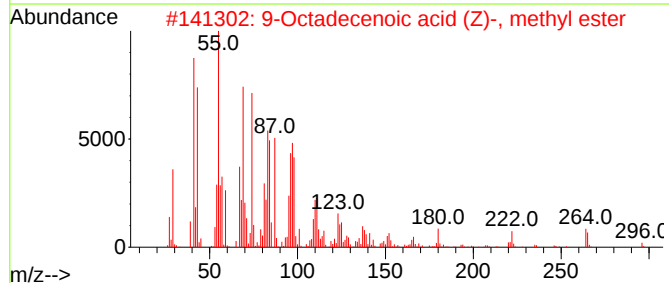
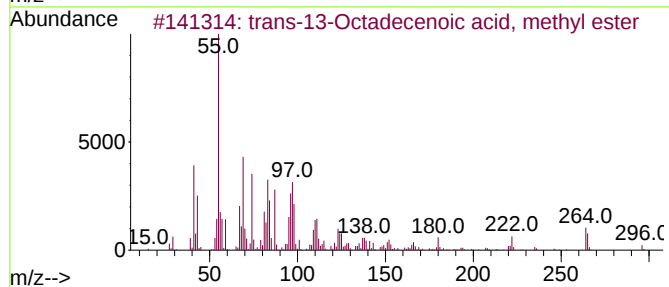
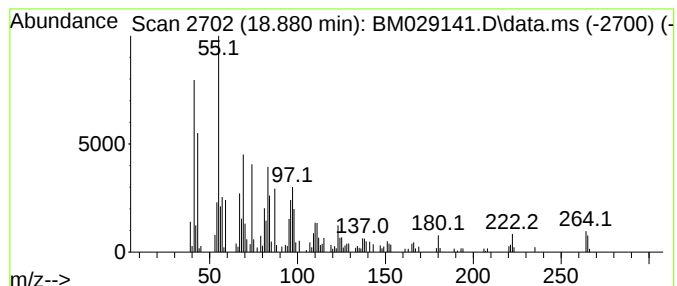
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Peak Number 4 trans-13-Octadecenoic acid,... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.880	33.30 ng	171986	Phenanthrene-d10	17.033	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	95
2	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	91
3	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	91
4	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	91
5	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	91



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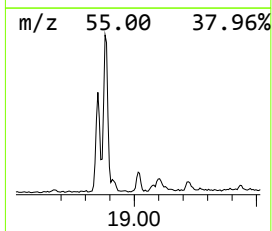
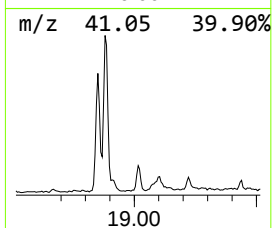
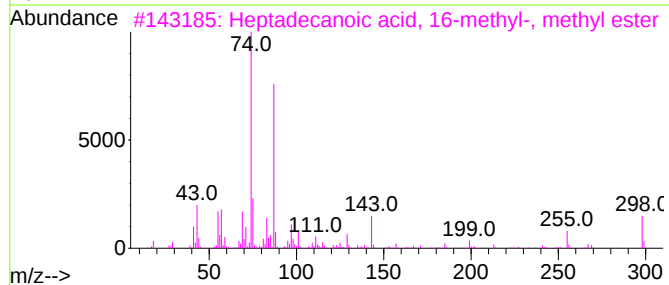
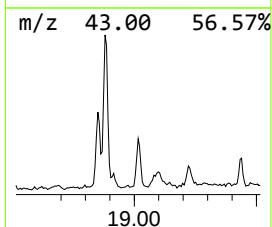
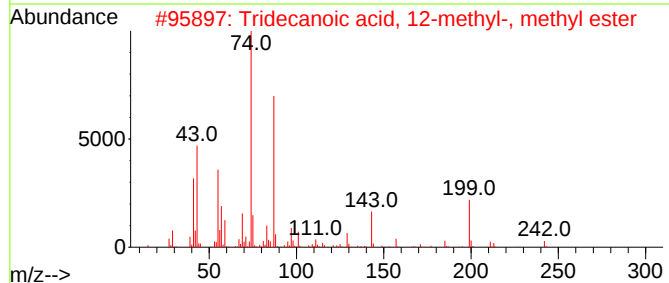
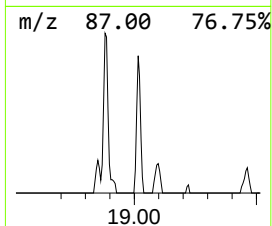
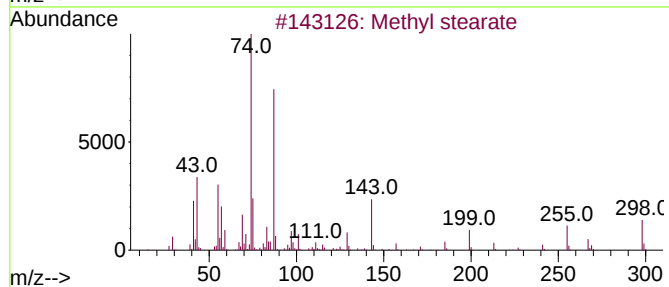
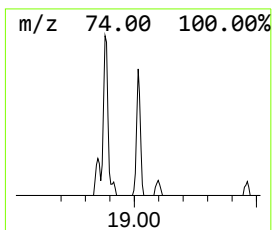
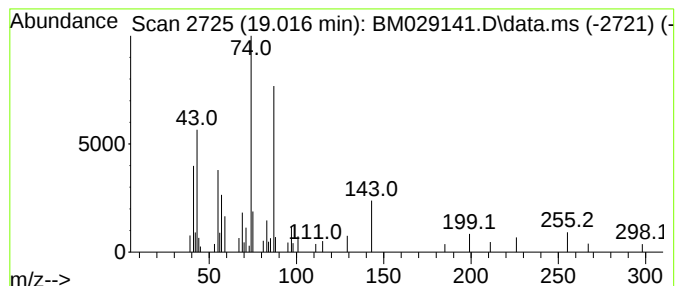
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Methyl stearate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.016	5.71 ng	29480	Phenanthrene-d10	17.033

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl stearate	298	C19H38O2	000112-61-8	97
2			Tridecanoic acid, 12-methyl-, me...	242	C15H30O2	005129-58-8	87
3			Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	83
4			Dodecanoic acid, 10-methyl-, met...	228	C14H28O2	005129-65-7	80
5			Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	80



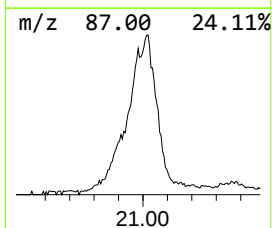
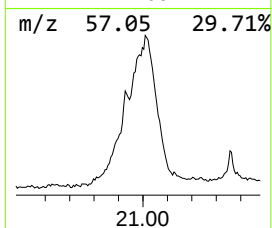
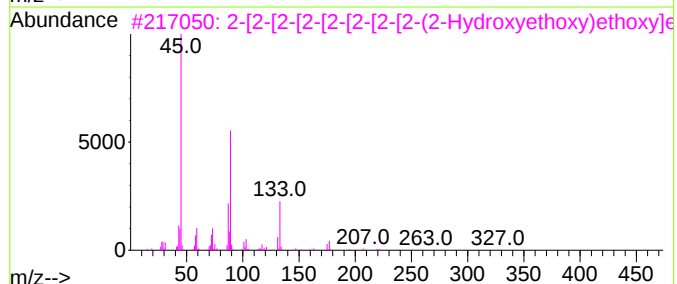
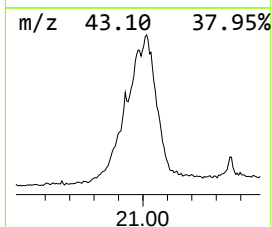
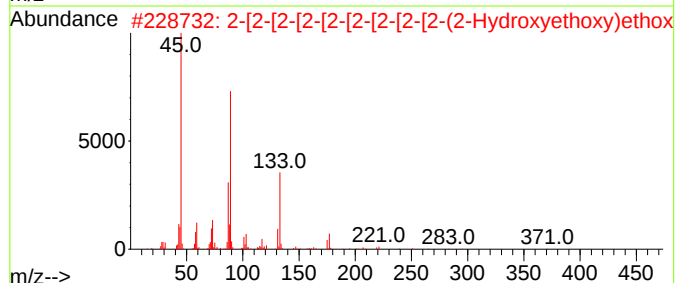
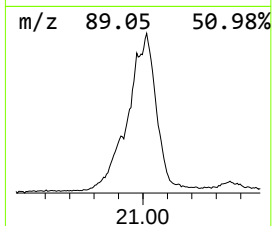
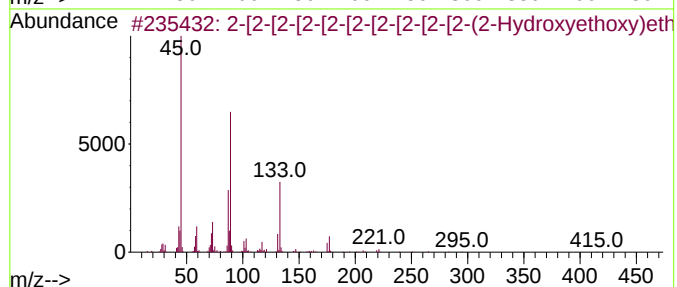
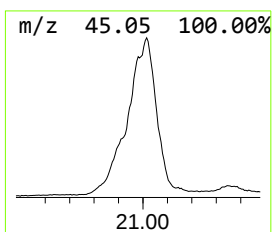
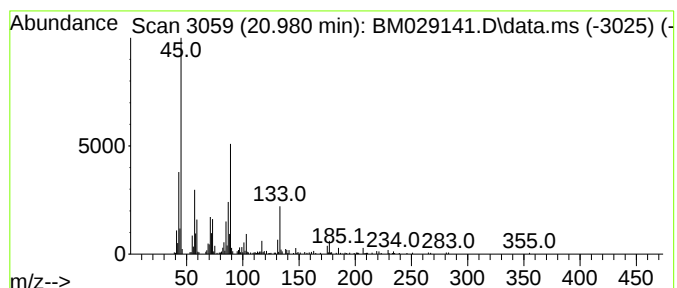
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Data File : BM029141.D  
Acq On    : 15 Mar 2021   21:51  
Operator   : CG/JU  
Sample     : M1668-01 5X  
Misc      :  
ALS Vial   : 17      Sample Multiplier: 1
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number	2-[2-[2-[2-[2-[2-[2-[2-[2-[...	Concentration Rank
6	2-[2-[2-[2-[2-[2-[2-[2-[2-[...	1

R.T.	EstConc	Area	Relative to ISTD		R.T.	
20.980	98.33 ng	811730	Chrysene-d12		21.215	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-[2-[2-[2-[2-[2-[2-[2-(2-...		502	C22H46O12	1000352-13-2	95
2	2-[2-[2-[2-[2-[2-[2-(2-Hyd...		458	C20H42O11	1000352-12-6	93
3	2-[2-[2-[2-[2-[2-(2-Hydrox...		414	C18H38O10	1000352-12-5	91
4	Heptaethylene glycol		326	C14H30O8	005617-32-3	91
5	2-[2-[2-[2-[2-[2-(2-Hydroxvet...		370	C16H34O9	005117-19-1	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM031521\
Data File : BM029141.D
Acq On : 15 Mar 2021 21:51
Operator : CG/JU
Sample : M1668-01 5X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
CL-02-031221

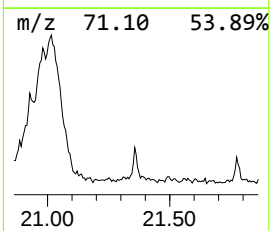
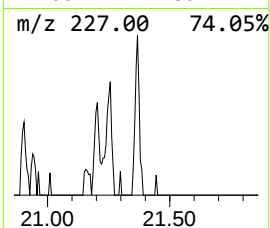
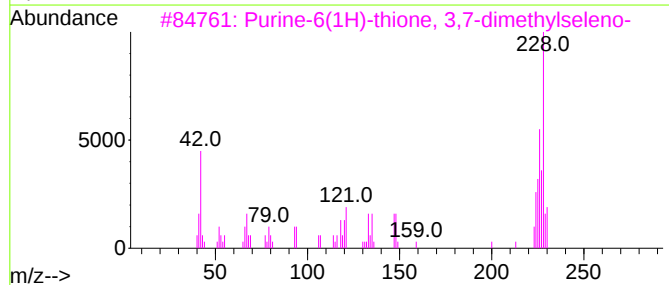
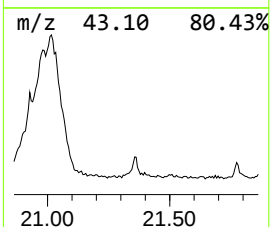
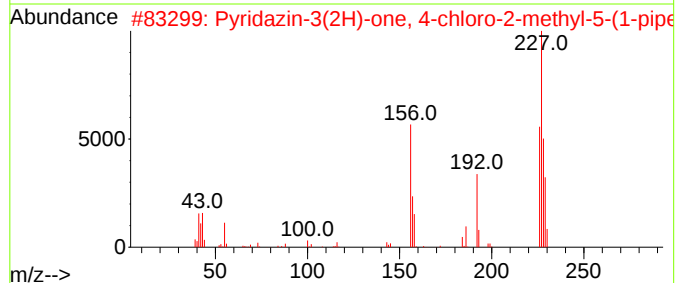
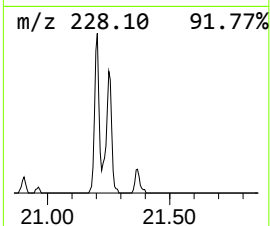
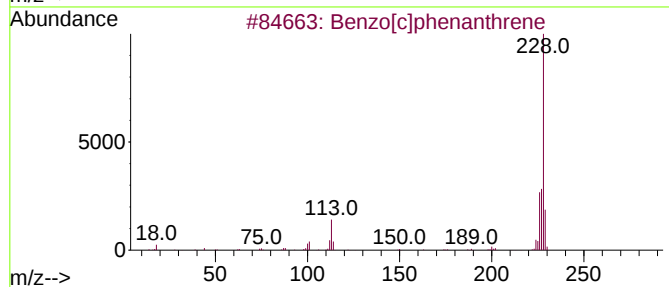
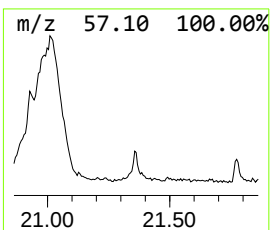
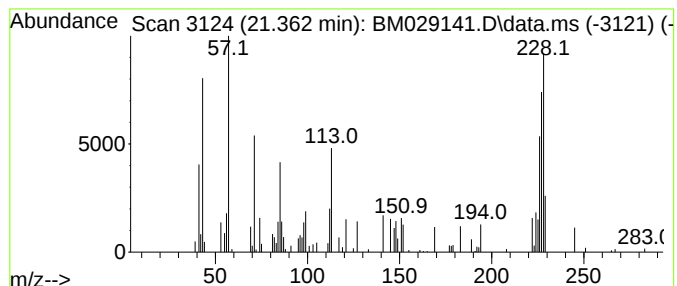
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown21.363 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.363	2.56 ng	21169	Chrysene-d12	21.215

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[c]phenanthrene	228	C18H12	000195-19-7	35
2			Pyridazin-3(2H)-one, 4-chloro-2...	227	C10H14ClN3O	001016-06-4	35
3			Purine-6(1H)-thione, 3,7-dimethy...	228	C7H8N4Se	023663-58-3	25
4			2-Thiazolamine, 4,5-dihydro-N-(1...	228	C13H12N2S	1000362-49-4	23
5			2,1,3-Benzoselenadiazole-5-carbo...	228	C7H4N2O2Se	140669-75-6	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM031521\
Data File : BM029141.D
Acq On : 15 Mar 2021 21:51
Operator : CG/JU
Sample : M1668-01 5X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
CL-02-031221

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Hexadecanoic ac...	17.704	9.8	ng	50820	4	17.033	103308	20.0
n-Decanoic acid	17.933	4.2	ng	21776	4	17.033	103308	20.0
9,12-Octadecadi...	18.851	28.4	ng	146576	4	17.033	103308	20.0
trans-13-Octade...	18.880	33.3	ng	171986	4	17.033	103308	20.0
Methyl stearate	19.016	5.7	ng	29480	4	17.033	103308	20.0
2-[2-[2-[2-[2-...	20.980	98.3	ng	811730	5	21.215	165110	20.0
unknown21.363	21.363	2.6	ng	21169	5	21.215	165110	20.0