

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM033023\
 Data File : BM039235.D
 Acq On : 30 Mar 2023 20:22
 Operator : CG/JU
 Sample : 02117-01
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 NB-8-032823

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-BM032923.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM039235.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	287	294	307	rVB	1551366	2190335	22.76%	3.476%
2	5.481	367	373	386	rBV	3650171	5204368	54.08%	8.260%
3	7.092	639	647	660	rBV	3431203	5329242	55.38%	8.458%
4	7.922	782	788	796	rVB	779825	1183794	12.30%	1.879%
5	9.092	979	987	999	rBV	2116025	3454301	35.90%	5.482%
6	10.733	1254	1266	1273	rBV	991782	1636678	17.01%	2.598%
7	12.192	1509	1514	1526	rVB	202532	314848	3.27%	0.500%
8	13.192	1677	1684	1694	rBV	5096080	7076483	73.54%	11.231%
9	14.568	1909	1918	1925	rBV	1405599	2026291	21.06%	3.216%
10	16.057	2163	2171	2178	rBV	3863097	5364727	55.75%	8.514%
11	16.274	2203	2208	2216	rBV5	58989	139173	1.45%	0.221%
12	16.421	2227	2233	2237	rBV2	66427	117799	1.22%	0.187%
13	17.315	2375	2385	2390	rBV	1682949	2360345	24.53%	3.746%
14	17.515	2410	2419	2426	rBV5	68840	156109	1.62%	0.248%
15	17.986	2494	2499	2504	rVB	244720	296958	3.09%	0.471%
16	18.209	2532	2537	2547	rBV	766410	1183220	12.30%	1.878%
17	19.127	2688	2693	2696	rBV	1173009	1422674	14.78%	2.258%
18	19.156	2696	2698	2707	rVB2	574073	724737	7.53%	1.150%
19	19.292	2717	2721	2724	rBV	112138	131663	1.37%	0.209%
20	19.368	2731	2734	2741	rVB2	106493	187781	1.95%	0.298%
21	19.486	2750	2754	2765	rBV	302496	497570	5.17%	0.790%
22	19.939	2826	2831	2840	rBV	7970665	9622687	100.00%	15.272%
23	20.244	2880	2883	2886	rVB	110523	111236	1.16%	0.177%
24	21.203	3042	3046	3055	rBV	1054267	1464214	15.22%	2.324%
25	21.497	3092	3096	3101	rBV	2058708	2691957	27.98%	4.272%
26	22.138	3198	3205	3214	rVB2	766676	1443110	15.00%	2.290%
27	22.862	3325	3328	3334	rVB2	330616	445073	4.63%	0.706%
28	23.168	3376	3380	3384	rVB	464304	690106	7.17%	1.095%
29	23.221	3385	3389	3400	rVB	785498	1504312	15.63%	2.388%
30	23.915	3501	3507	3522	rVB2	1462408	2941899	30.57%	4.669%
31	24.521	3605	3610	3619	rVB	528097	1094003	11.37%	1.736%

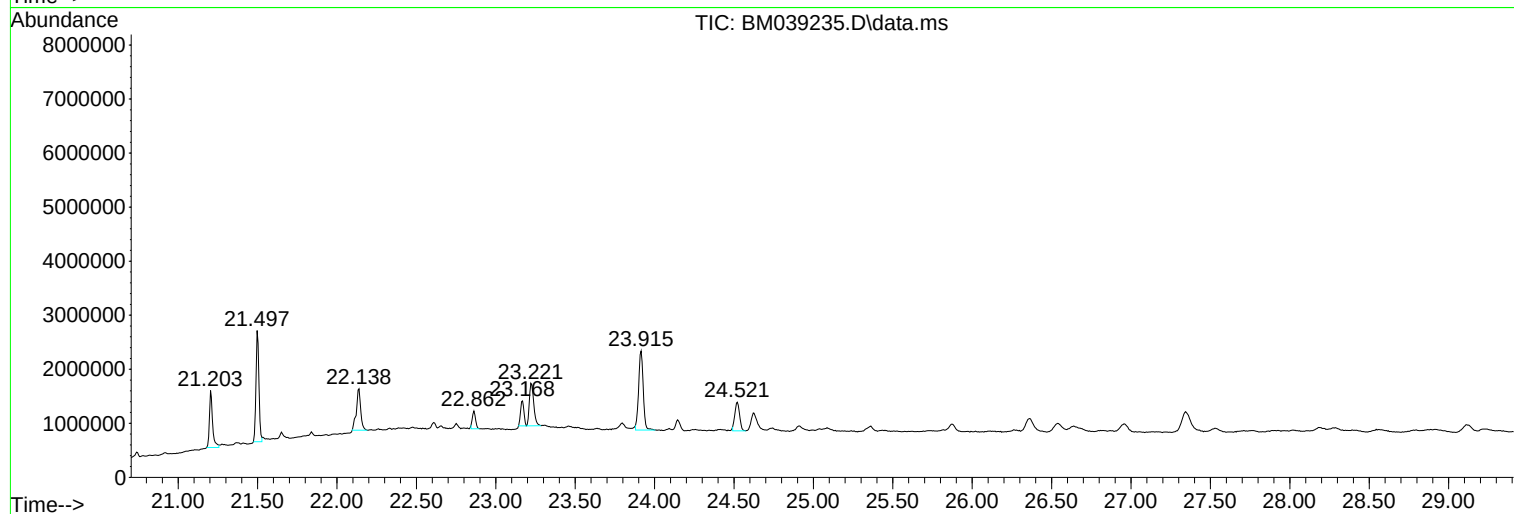
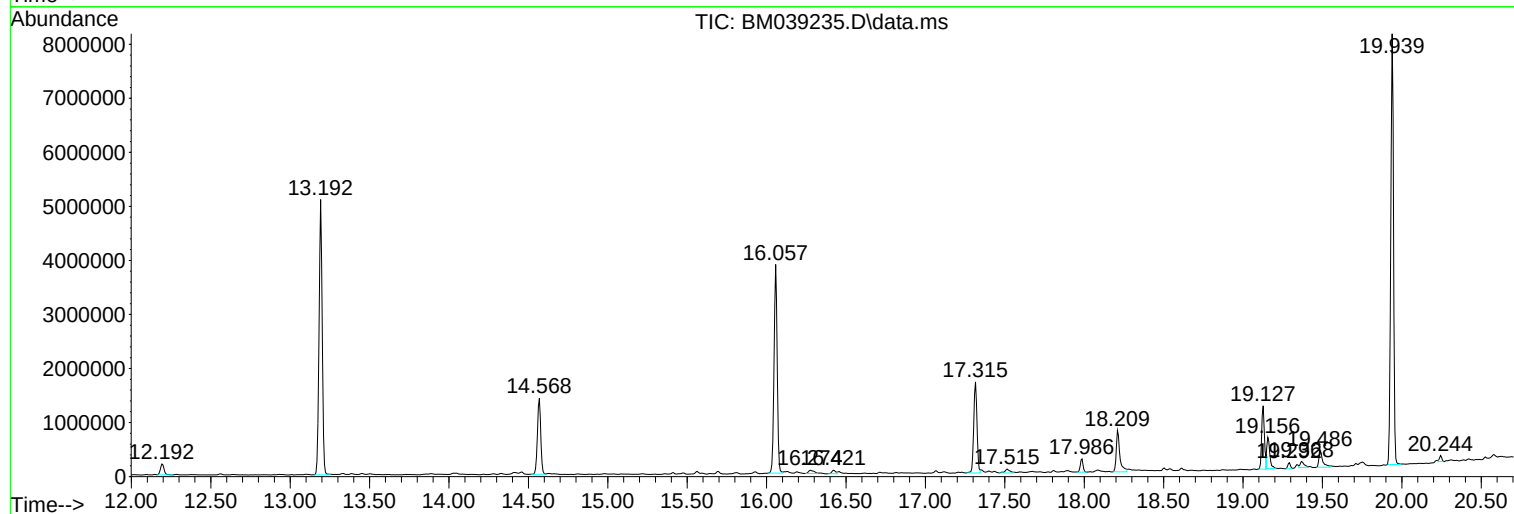
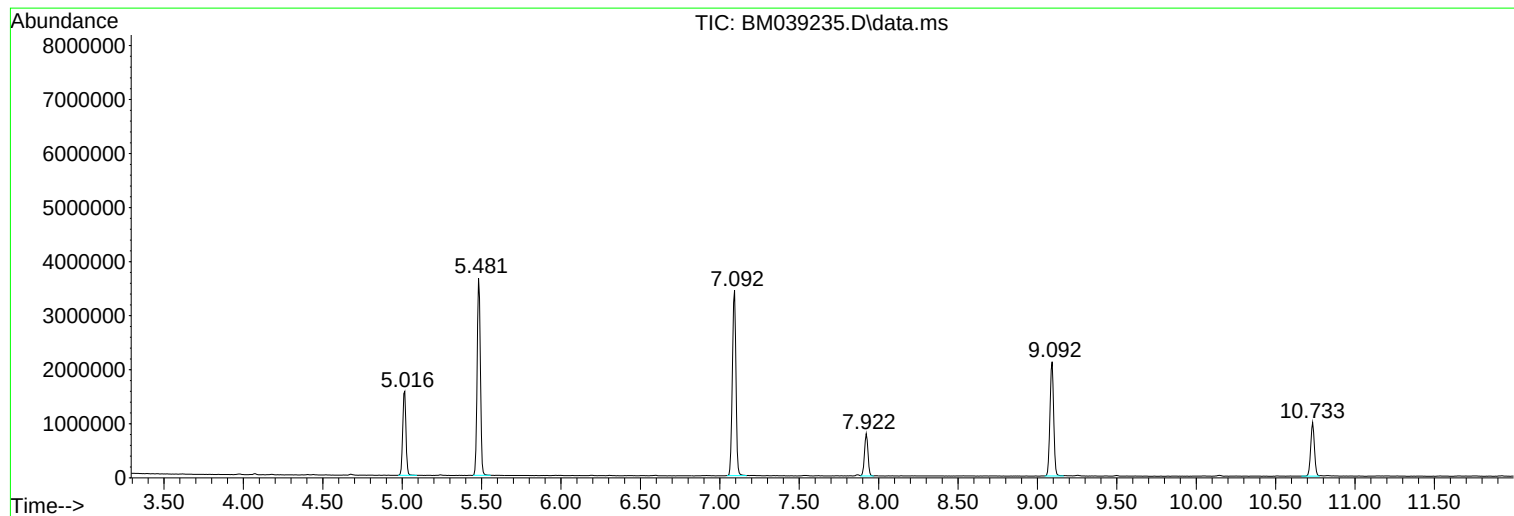
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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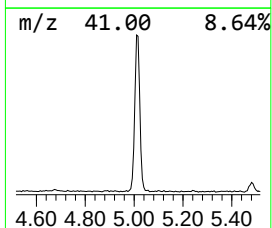
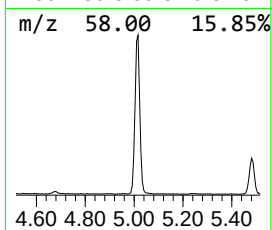
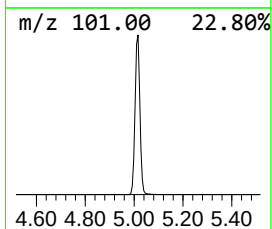
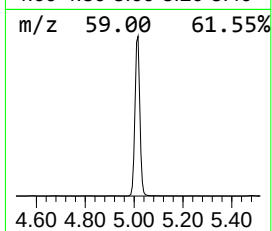
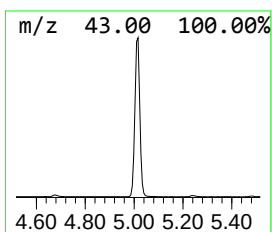
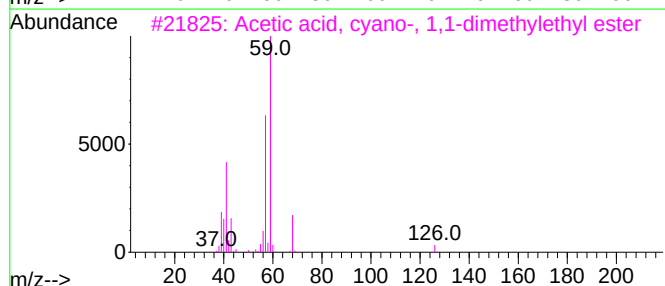
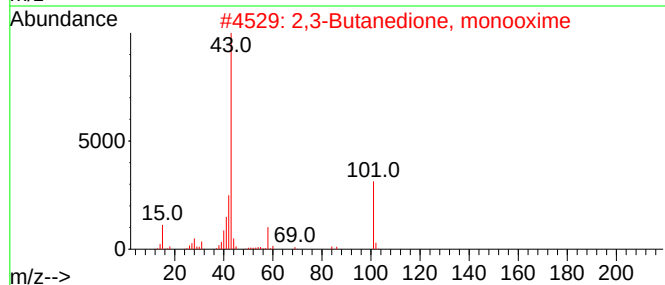
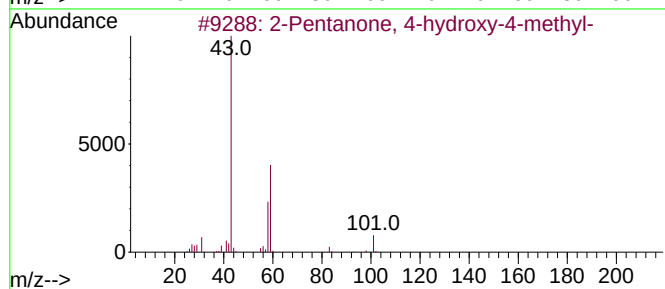
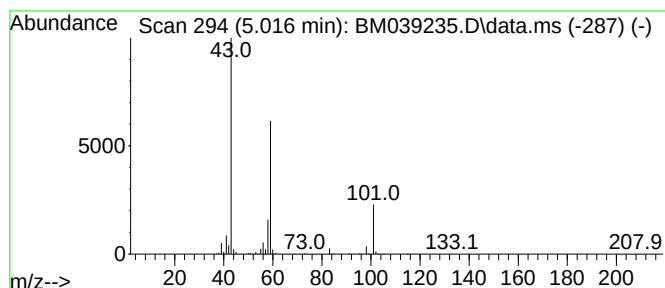
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TIC Library : C:\Database\NIST20.L
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.016	37.01 ng	2190340	1,4-Dichlorobenzene-d4	7.922

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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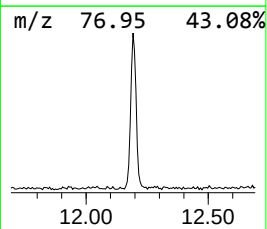
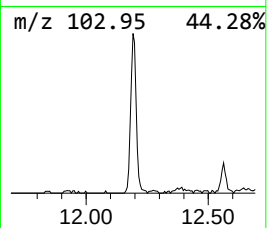
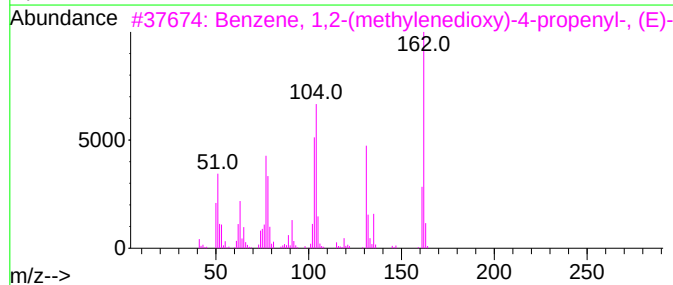
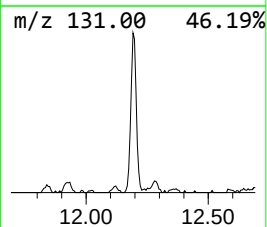
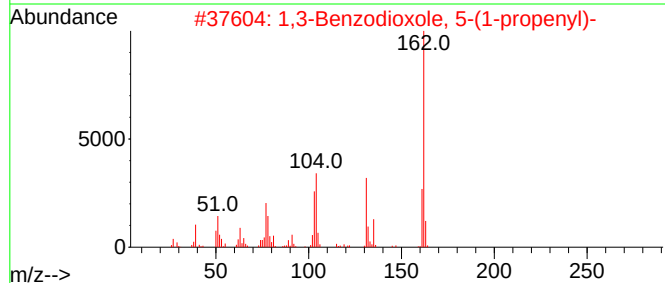
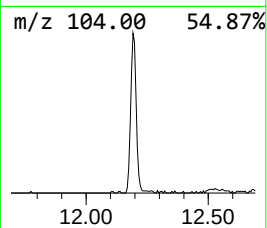
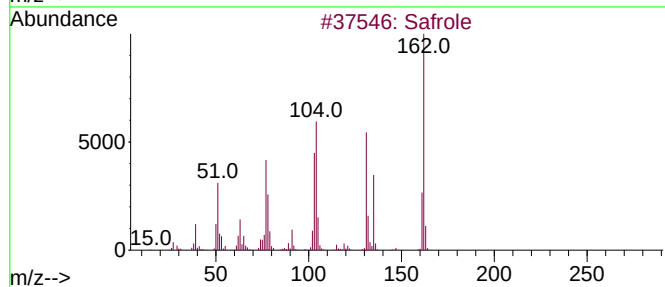
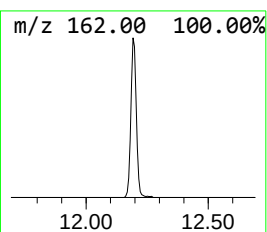
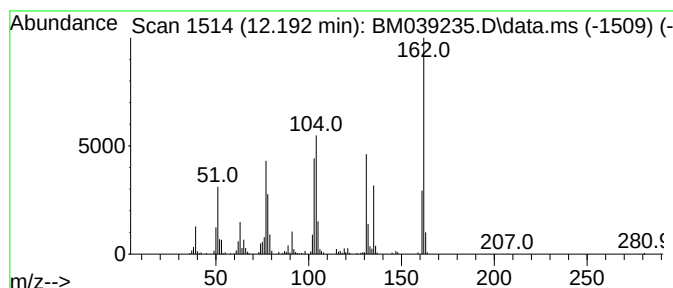
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Peak Number 2 Safrole Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.192	3.85 ng	314848	Naphthalene-d8	10.733

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Safrole	162	C10H10O2	000094-59-7	98
2			1,3-Benzodioxole, 5-(1-propenyl)-	162	C10H10O2	000120-58-1	97
3			Benzene, 1,2-(methylenedioxy)-4-...	162	C10H10O2	004043-71-4	94
4			1,3-Benzodioxole, 5-(1-propenyl)...	162	C10H10O2	017627-76-8	94
5			1H-Isoindole-1,3(2H)-dione, 2-am...	162	C8H6N2O2	001875-48-5	46



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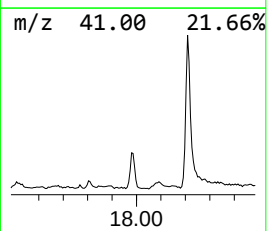
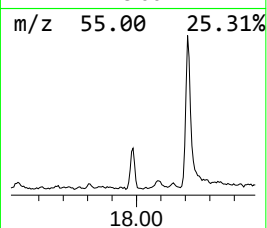
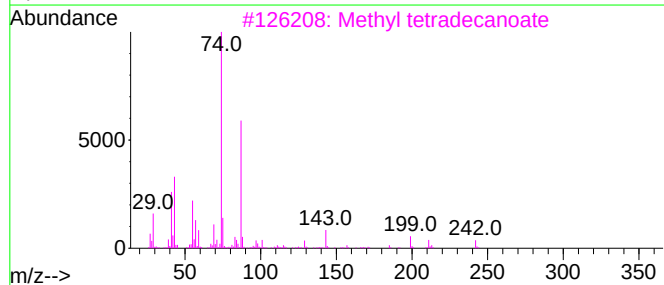
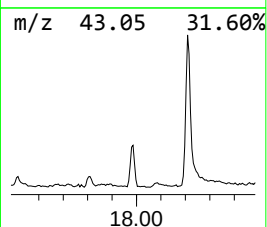
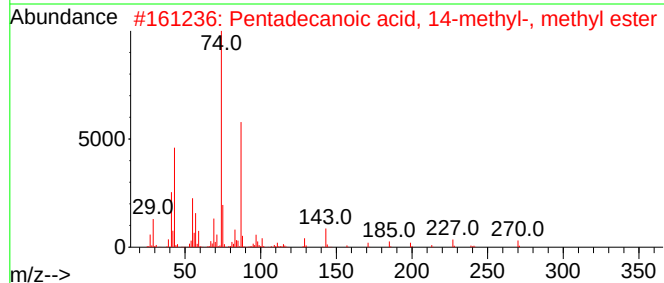
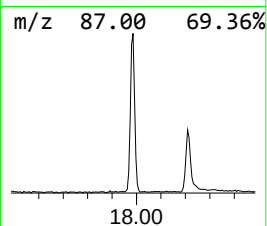
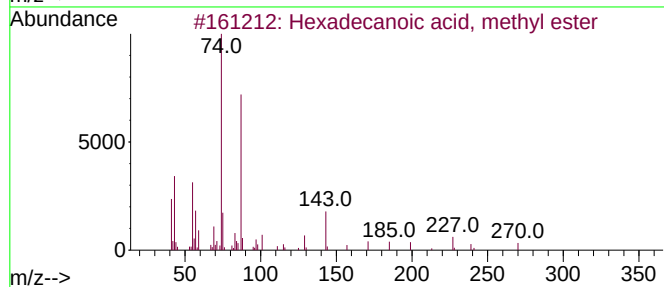
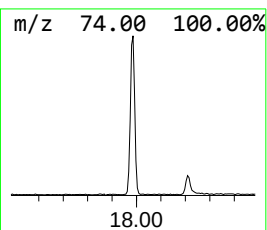
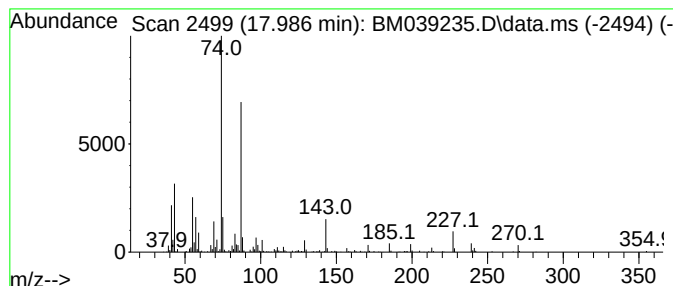
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Peak Number 3 Hexadecanoic acid, methyl e... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD		R.T.	
17.986	2.52 ng	296958	Phenanthrene-d10		17.315	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester		270	C17H34O2	000112-39-0	99
2	Pentadecanoic acid, 14-methyl-, ...		270	C17H34O2	005129-60-2	97
3	Methyl tetradecanoate		242	C15H30O2	000124-10-7	93
4	Tridecanoic acid, methyl ester		228	C14H28O2	001731-88-0	91
5	Hexadecanoic acid, 2-methyl-		270	C17H34O2	027147-71-3	87



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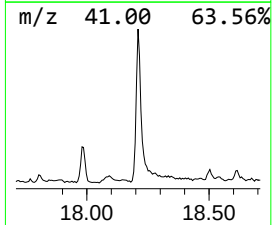
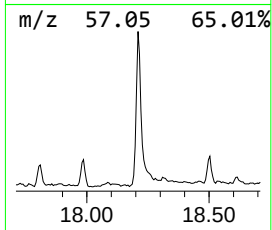
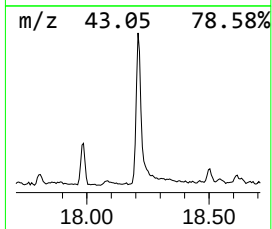
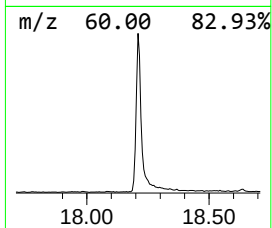
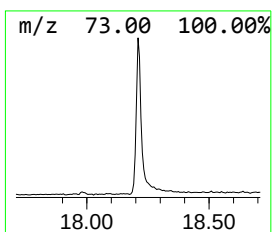
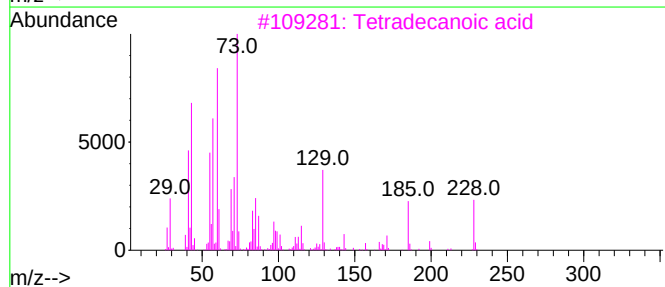
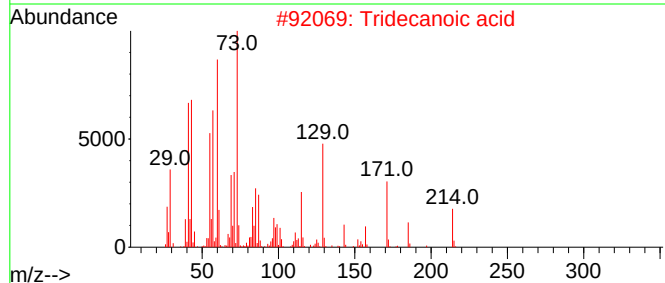
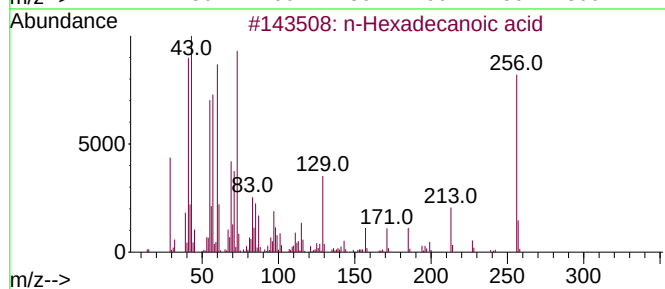
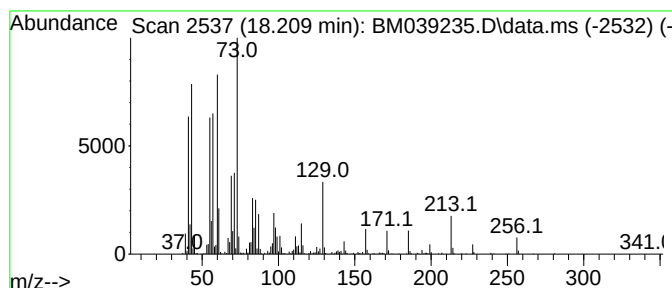
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.209	10.03 ng	1183220	Phenanthrene-d10	17.315

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	94
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	93
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
5			Isopropyl palmitate	298	C19H38O2	000142-91-6	53



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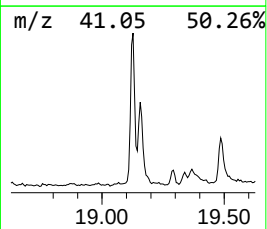
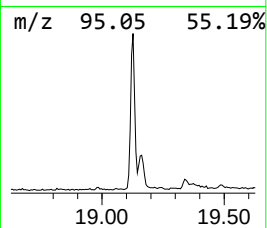
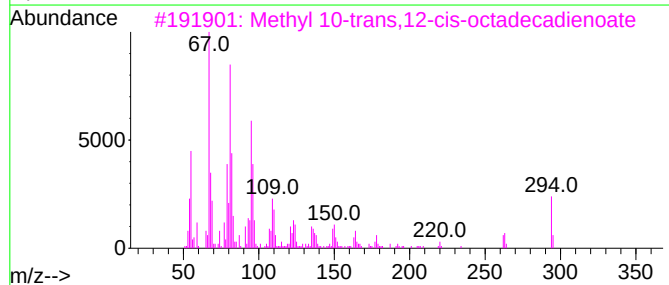
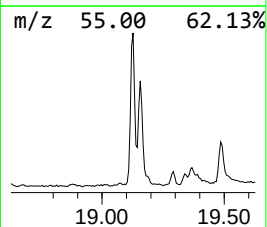
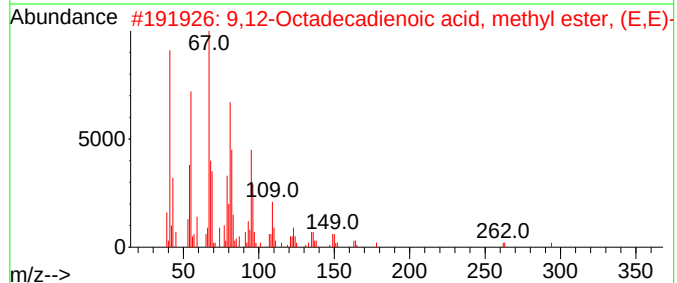
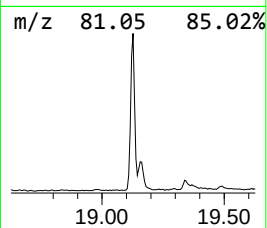
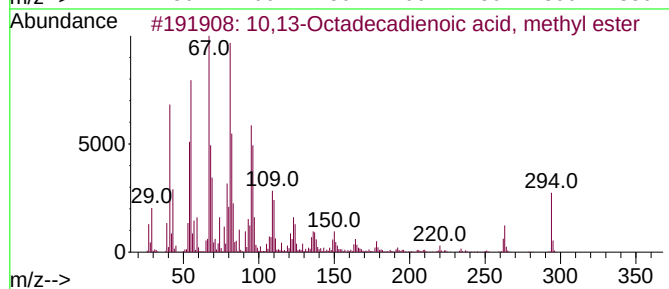
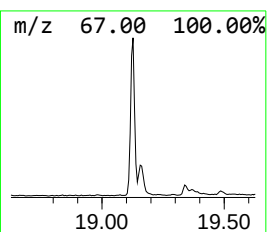
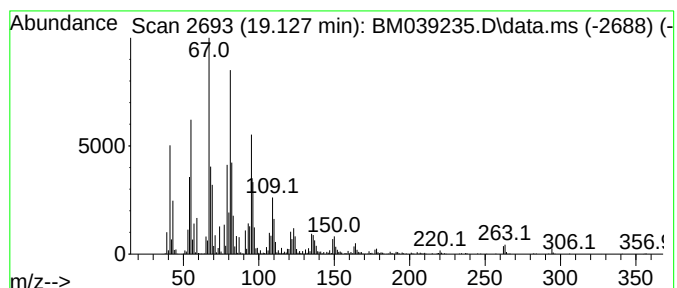
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Peak Number 5 10,13-Octadecadienoic acid,... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.127	12.05 ng	1422670	Phenanthrene-d10	17.315	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	99
2	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
3	Methyl 10-trans,12-cis-octadecad...	294	C19H34O2	1000336-44-2	99
4	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99
5	8,11-Octadecadienoic acid, methy...	294	C19H34O2	056599-58-7	99



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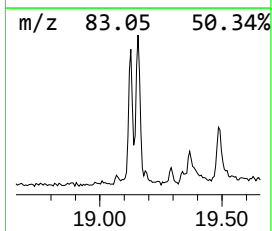
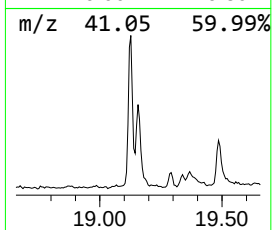
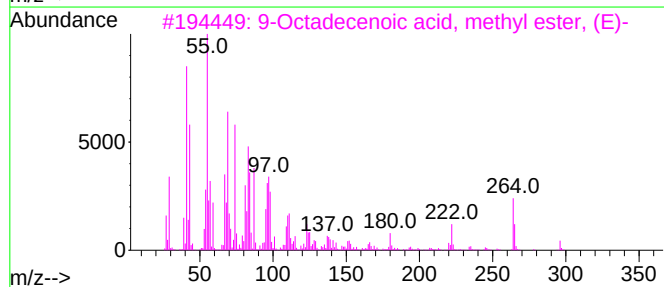
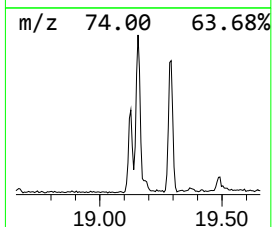
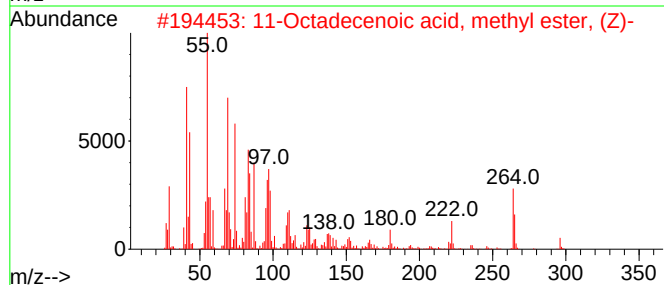
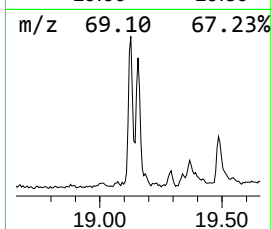
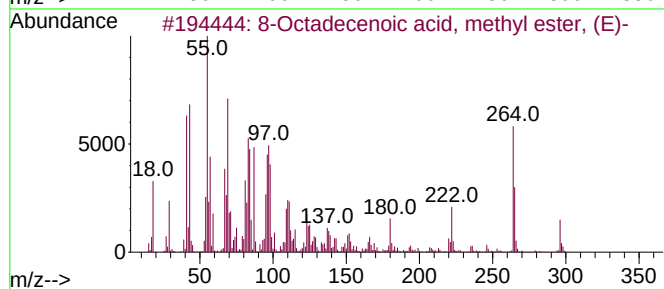
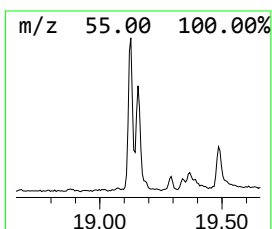
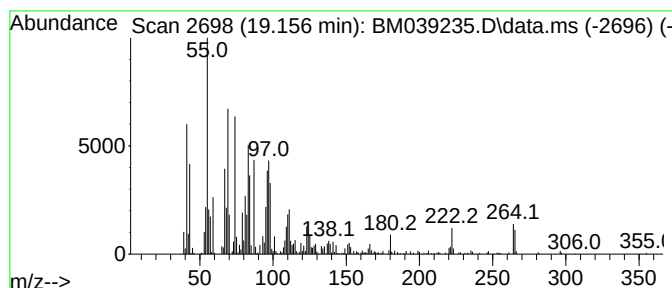
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 8-Octadecenoic acid, methyl... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.156	6.14 ng	724737	Phenanthrene-d10	17.315	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	8-Octadecenoic acid, methyl este...	296	C19H36O2	026528-50-7	99
2	11-Octadecenoic acid, methyl est...	296	C19H36O2	001937-63-9	99
3	9-Octadecenoic acid, methyl este...	296	C19H36O2	001937-62-8	99
4	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	99
5	9-Octadecenoic acid, methyl ester	296	C19H36O2	002462-84-2	99



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM033023\
Data File : BM039235.D
Acq On : 30 Mar 2023 20:22
Operator : CG/JU
Sample : 02117-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
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ClientSampleId :
NB-8-032823

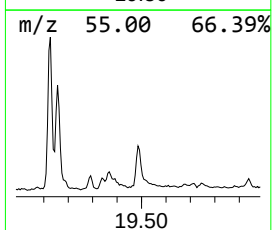
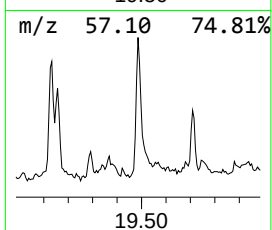
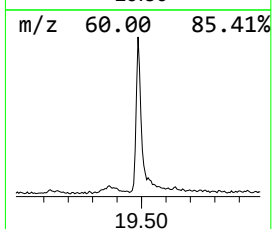
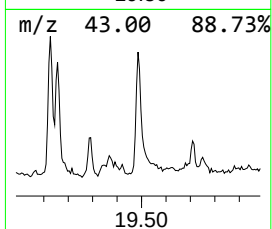
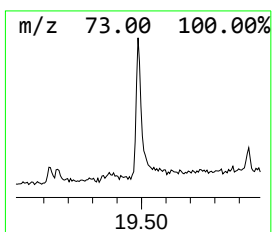
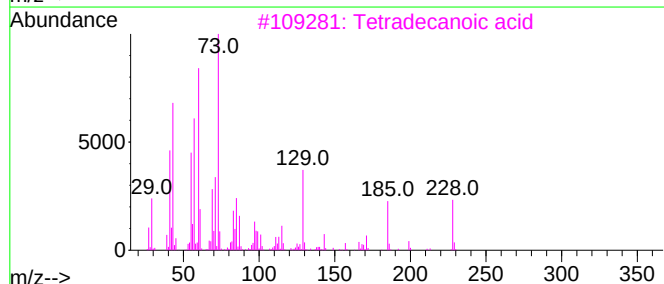
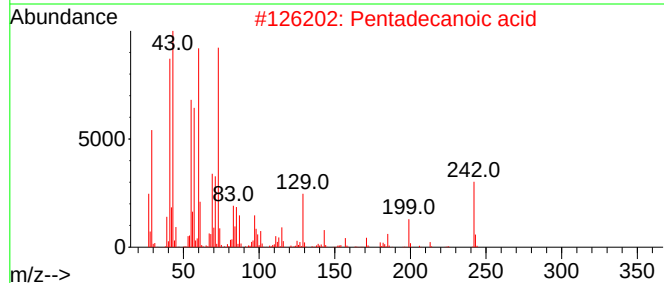
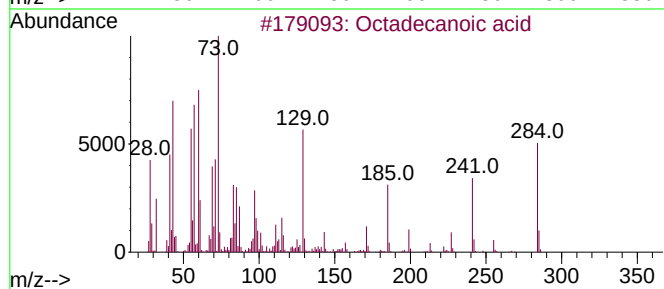
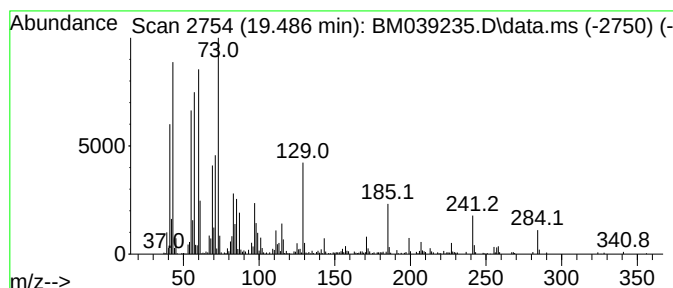
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.486	3.70 ng	497570	Chrysene-d12	21.497

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	93
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	90
4			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	80
5			n-Decanoic acid	172	C10H20O2	000334-48-5	68



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM033023\
Data File : BM039235.D
Acq On : 30 Mar 2023 20:22
Operator : CG/JU
Sample : 02117-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

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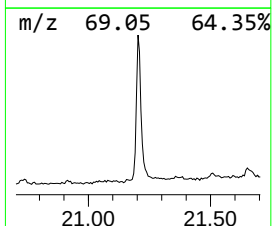
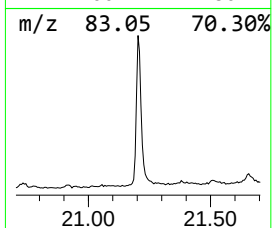
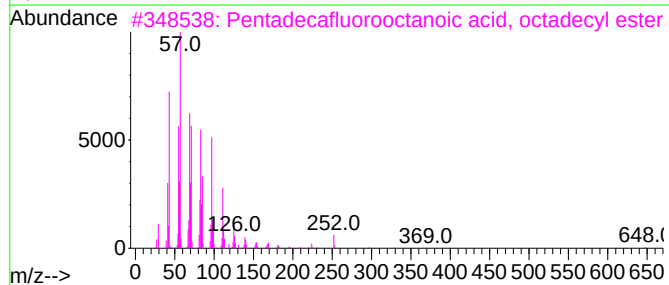
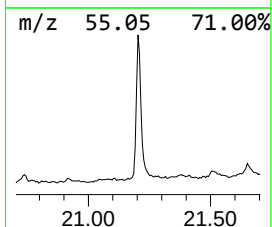
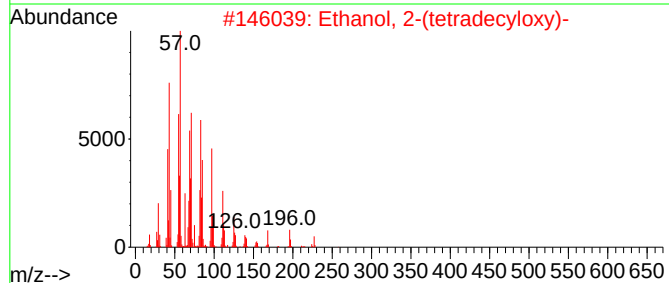
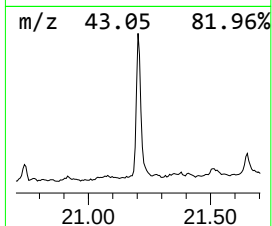
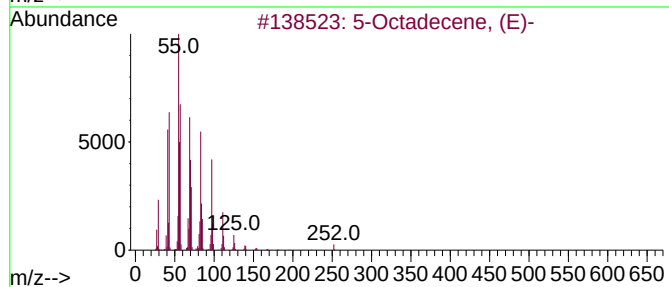
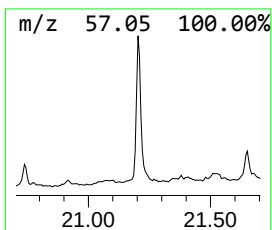
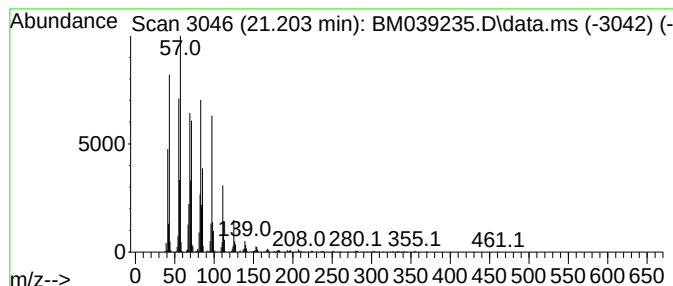
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 5-Octadecene, (E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.203	10.88 ng	1464210	Chrysene-d12	21.497

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Octadecene, (E)-	252	C18H36	007206-21-5	95
2			Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	95
3			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
4			1-Heneicosanol	312	C21H44O	015594-90-8	93
5			Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM033023\
Data File : BM039235.D
Acq On : 30 Mar 2023 20:22
Operator : CG/JU
Sample : 02117-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

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ClientSampleId :
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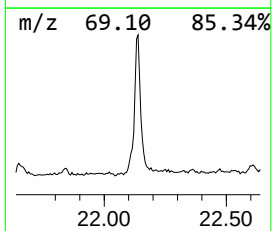
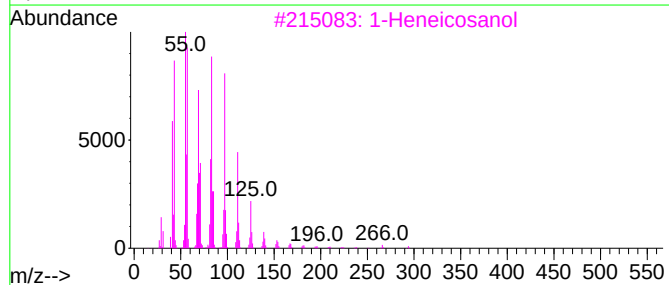
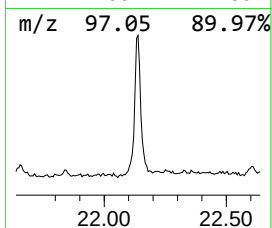
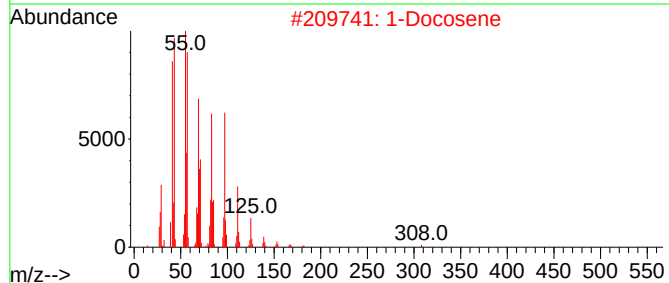
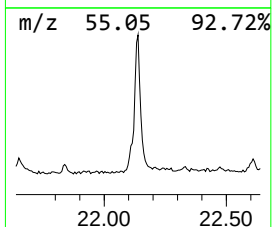
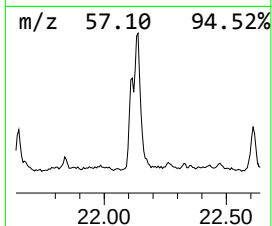
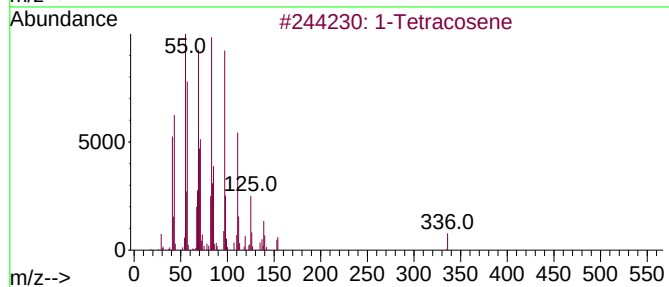
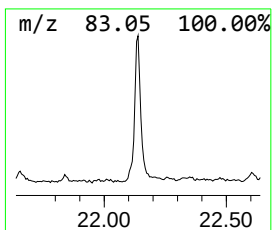
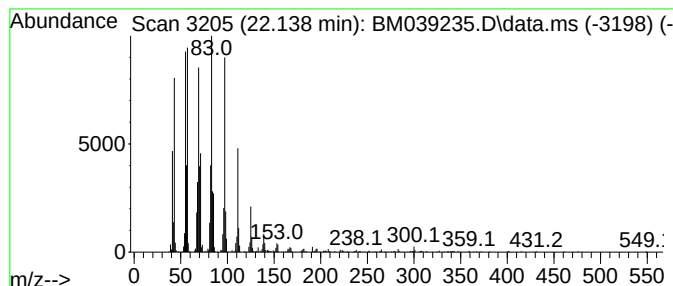
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1-Tetracosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.139	10.72 ng	1443110	Chrysene-d12	21.497

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Tetracosene	336	C24H48	010192-32-2	99
2			1-Docosene	308	C22H44	001599-67-3	97
3			1-Heneicosanol	312	C21H44O	015594-90-8	95
4			n-Tetracosanol-1	354	C24H50O	000506-51-4	94
5			n-Nonadecanol-1	284	C19H40O	001454-84-8	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM033023\
Data File : BM039235.D
Acq On : 30 Mar 2023 20:22
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Sample : 02117-01
Misc :
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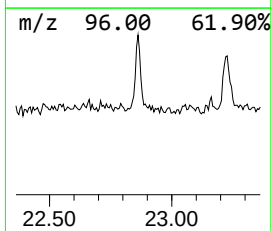
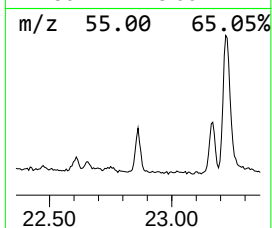
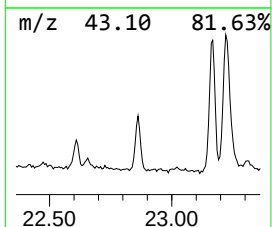
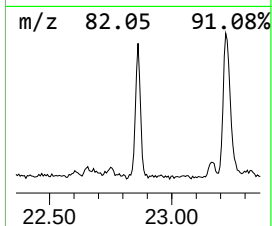
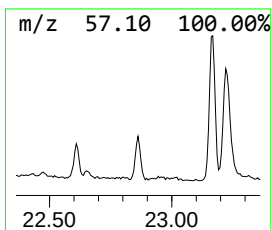
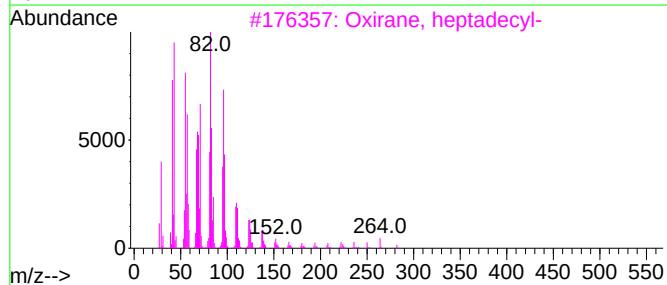
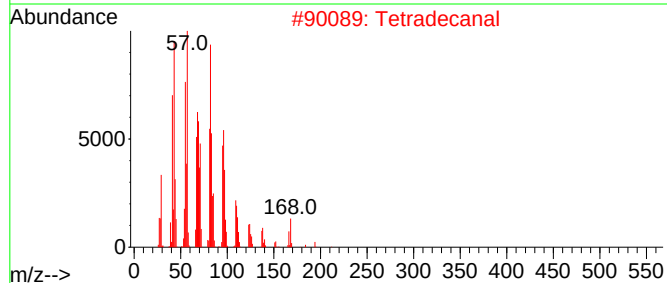
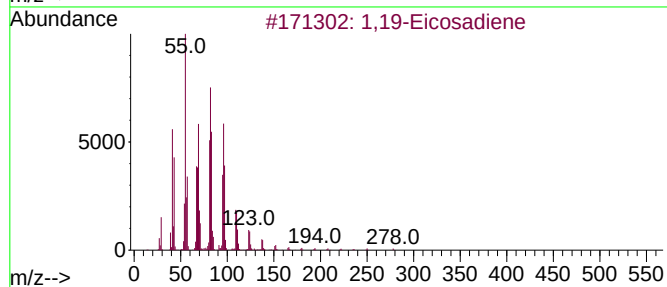
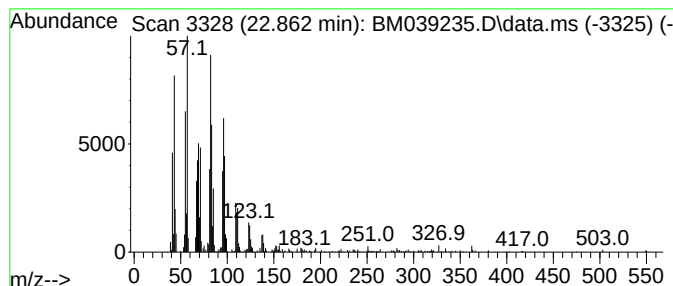
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 1,19-Eicosadiene Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.862	3.03 ng	445073	Perylene-d12	23.915

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,19-Eicosadiene	278	C20H38	014811-95-1	93
2			Tetradecanal	212	C14H28O	000124-25-4	93
3			Oxirane, heptadecyl-	282	C19H38O	067860-04-2	93
4			Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91
5			Octadecanal	268	C18H36O	000638-66-4	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM033023\
Data File : BM039235.D
Acq On : 30 Mar 2023 20:22
Operator : CG/JU
Sample : 02117-01
Misc :
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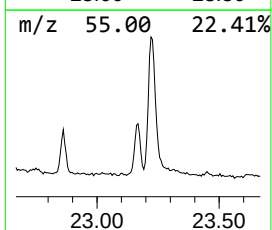
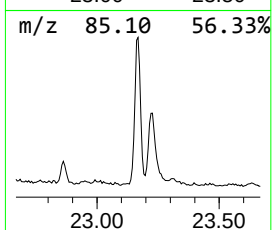
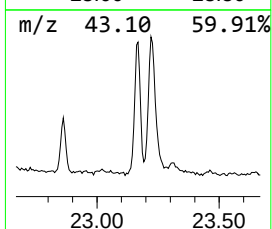
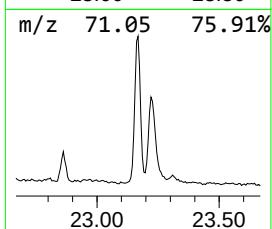
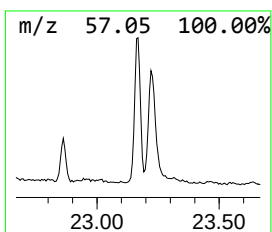
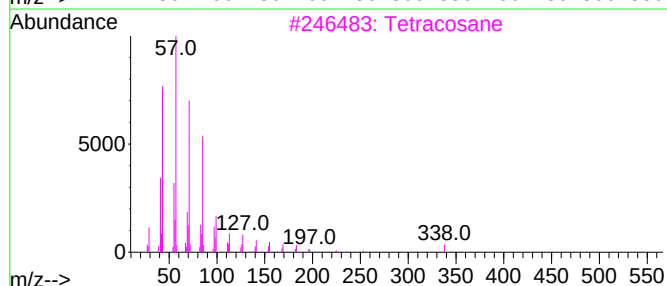
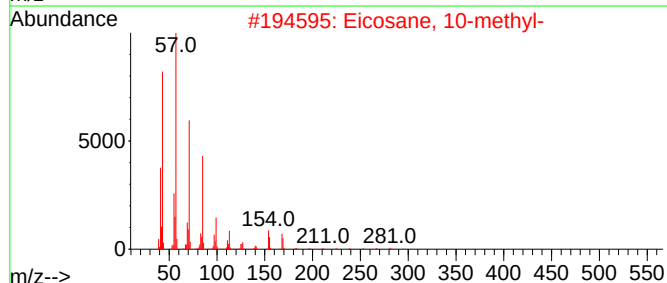
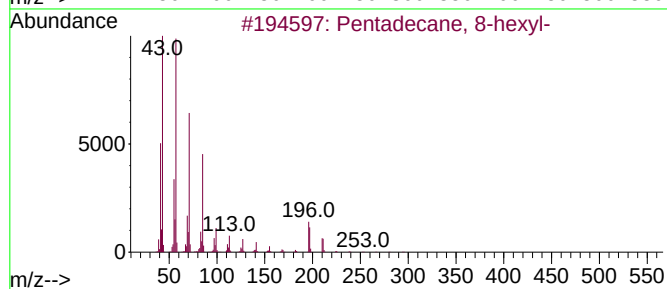
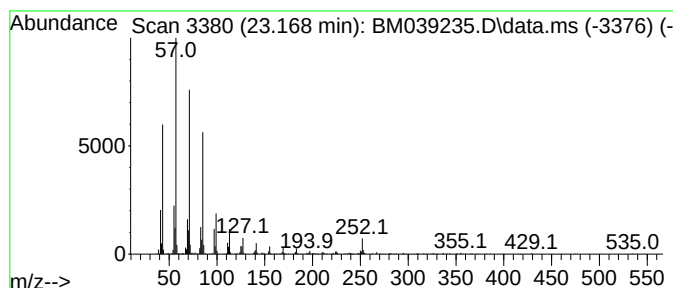
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Pentadecane, 8-hexyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
23.168	4.69 ng	690106	Perylene-d12	23.915	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	93
2	Eicosane, 10-methyl-	296	C21H44	054833-23-7	93
3	Tetracosane	338	C24H50	000646-31-1	90
4	Octacosane, 2-methyl-	408	C29H60	001560-98-1	90
5	Heneicosane	296	C21H44	000629-94-7	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM033023\
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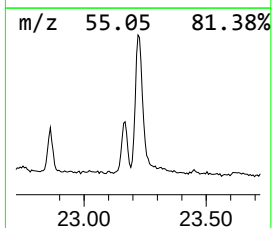
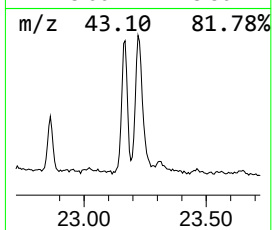
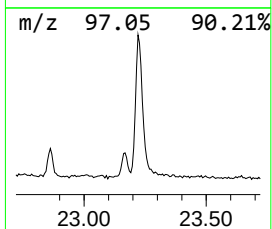
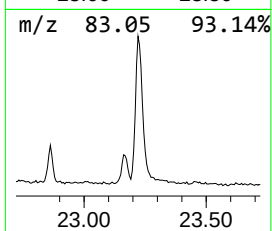
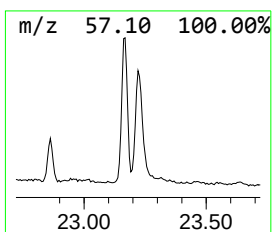
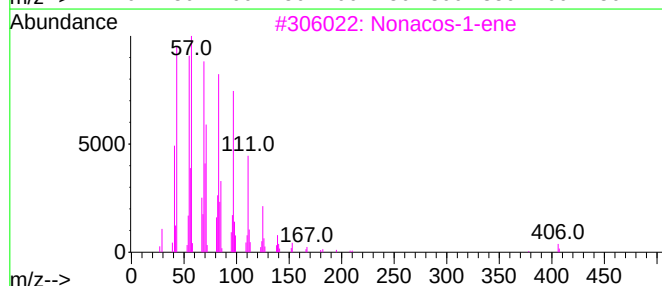
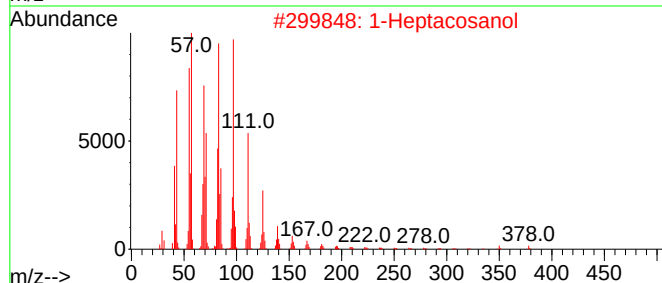
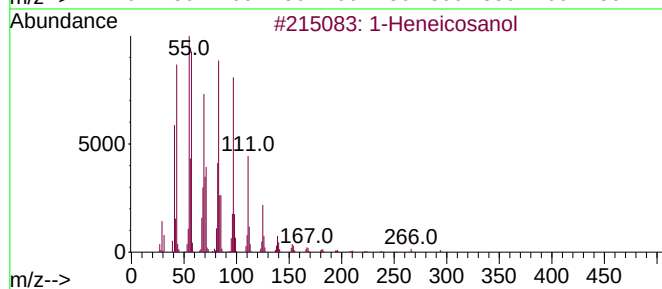
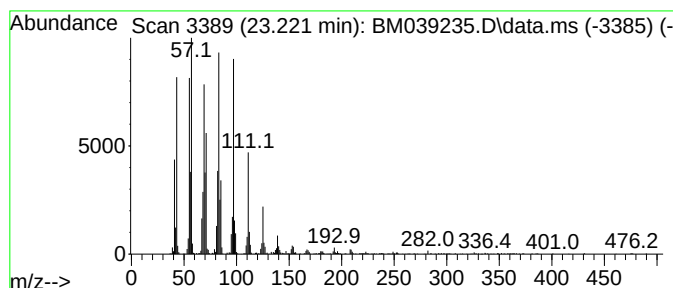
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
23.221	10.23 ng	1504310	Perylene-d12		23.915	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	1-Heneicosanol		312	C21H44O	015594-90-8	95
2	1-Heptacosanol		396	C27H56O	002004-39-9	95
3	Nonacos-1-ene		406	C29H58	018835-35-3	94
4	1-Hexacosene		364	C26H52	018835-33-1	94
5	Behenic alcohol		326	C22H46O	000661-19-8	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM033023\
Data File : BM039235.D
Acq On : 30 Mar 2023 20:22
Operator : CG/JU
Sample : 02117-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
NB-8-032823

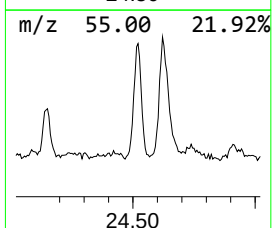
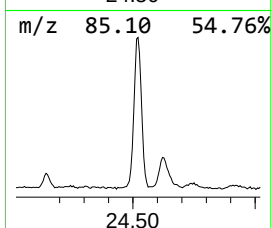
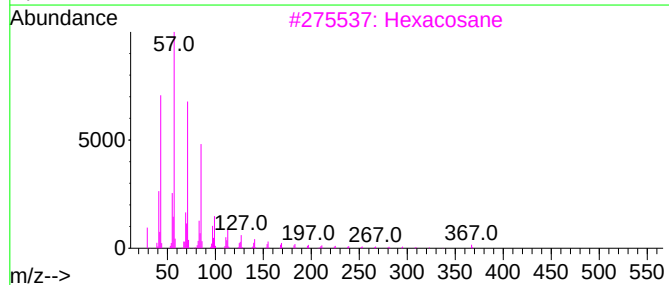
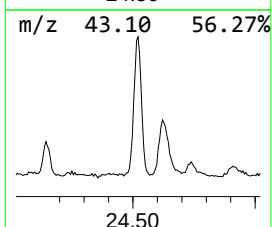
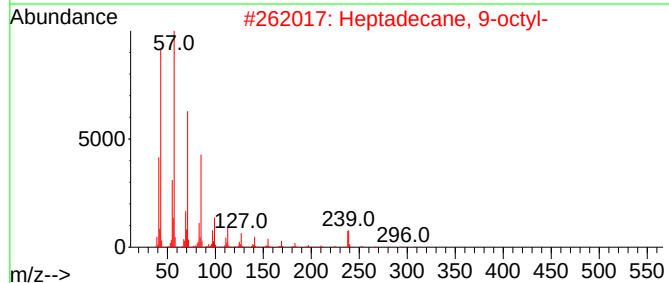
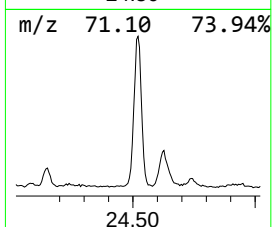
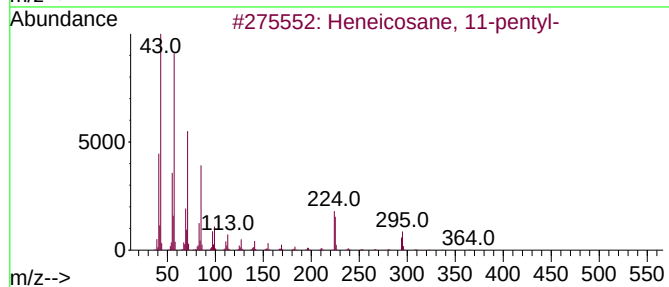
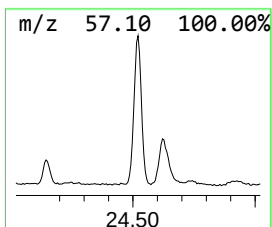
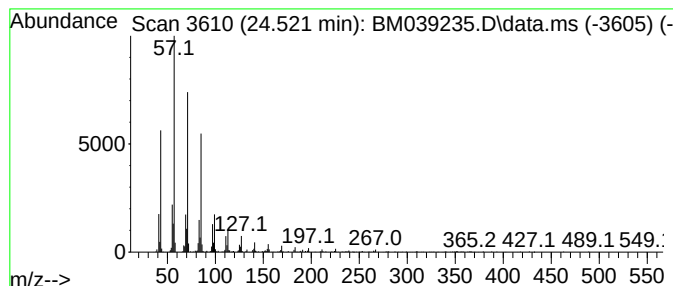
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Heneicosane, 11-pentyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.521	7.44 ng	1094000	Perylene-d12	23.915

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane, 11-pentyl-	366	C26H54	014739-72-1	94
2			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
3			Hexacosane	366	C26H54	000630-01-3	91
4			Tetracosane	338	C24H50	000646-31-1	91
5			Octacosane	394	C28H58	000630-02-4	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM033023\
Data File : BM039235.D
Acq On : 30 Mar 2023 20:22
Operator : CG/JU
Sample : 02117-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
NB-8-032823

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.016	37.0	ng	2190340	1	7.922	1183790	20.0
Safrrole	12.192	3.9	ng	314848	2	10.733	1636680	20.0
Hexadecanoic ac...	17.986	2.5	ng	296958	4	17.315	2360350	20.0
n-Hexadecanoic ...	18.209	10.0	ng	1183220	4	17.315	2360350	20.0
10,13-Octadecad...	19.127	12.1	ng	1422670	4	17.315	2360350	20.0
8-Octadecenoic ...	19.156	6.1	ng	724737	4	17.315	2360350	20.0
Octadecanoic acid	19.486	3.7	ng	497570	5	21.497	2691960	20.0
5-Octadecene, (E)-	21.203	10.9	ng	1464210	5	21.497	2691960	20.0
1-Tetracosene	22.139	10.7	ng	1443110	5	21.497	2691960	20.0
1,19-Eicosadiene	22.862	3.0	ng	445073	6	23.915	2941900	20.0
Pentadecane, 8-...	23.168	4.7	ng	690106	6	23.915	2941900	20.0
1-Heneicosanol	23.221	10.2	ng	1504310	6	23.915	2941900	20.0
Heneicosane, 11...	24.521	7.4	ng	1094000	6	23.915	2941900	20.0