

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121021\
 Data File : BM033406.D
 Acq On : 10 Dec 2021 22:14
 Operator : CG/JU
 Sample : M4927-04
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 PH1-BOT-6

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-BM120821.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM033406.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.490	378	383	395	rVB	842438	1237694	27.66%	5.401%
2	7.078	647	653	663	rVB	1460060	2341734	52.34%	10.218%
3	7.901	788	793	801	rVB	347947	561416	12.55%	2.450%
4	9.066	984	991	1003	rVB	1217713	2011717	44.96%	8.778%
5	10.695	1261	1268	1277	rBV	423835	735048	16.43%	3.207%
6	13.154	1679	1686	1696	rBV	2650534	3931460	87.87%	17.155%
7	14.524	1913	1919	1928	rVB	560946	861806	19.26%	3.761%
8	16.013	2161	2172	2187	rBV	1406778	2085582	46.62%	9.101%
9	17.265	2379	2385	2392	rBV	602417	892915	19.96%	3.896%
10	18.148	2530	2535	2540	rBV2	66083	94207	2.11%	0.411%
11	19.877	2823	2829	2835	rBV	3617893	4473997	100.00%	19.523%
12	21.124	3038	3041	3050	rBV4	149907	232346	5.19%	1.014%
13	21.430	3088	3093	3105	rBV	722521	961835	21.50%	4.197%
14	23.747	3481	3487	3496	rVB	413609	846444	18.92%	3.694%
15	24.283	3574	3578	3586	rVB	158140	290318	6.49%	1.267%
16	25.065	3707	3711	3718	rVB2	155476	329960	7.38%	1.440%
17	25.988	3862	3868	3875	rBV	180362	413945	9.25%	1.806%
18	27.071	4048	4052	4064	rVB2	234262	614210	13.73%	2.680%

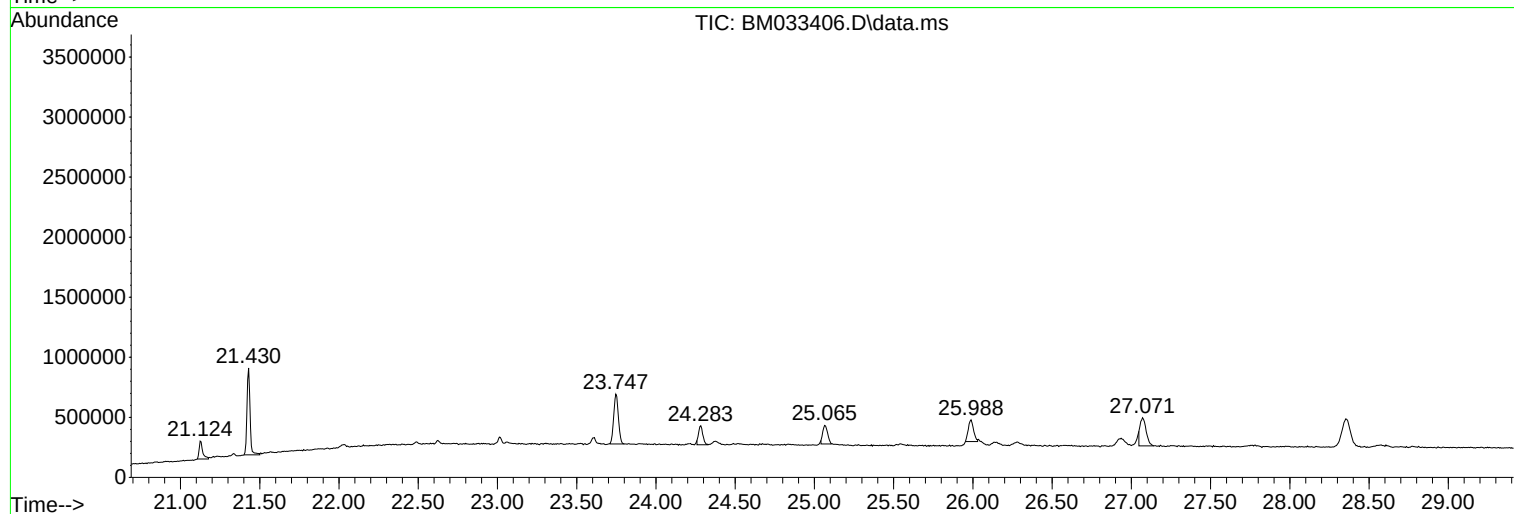
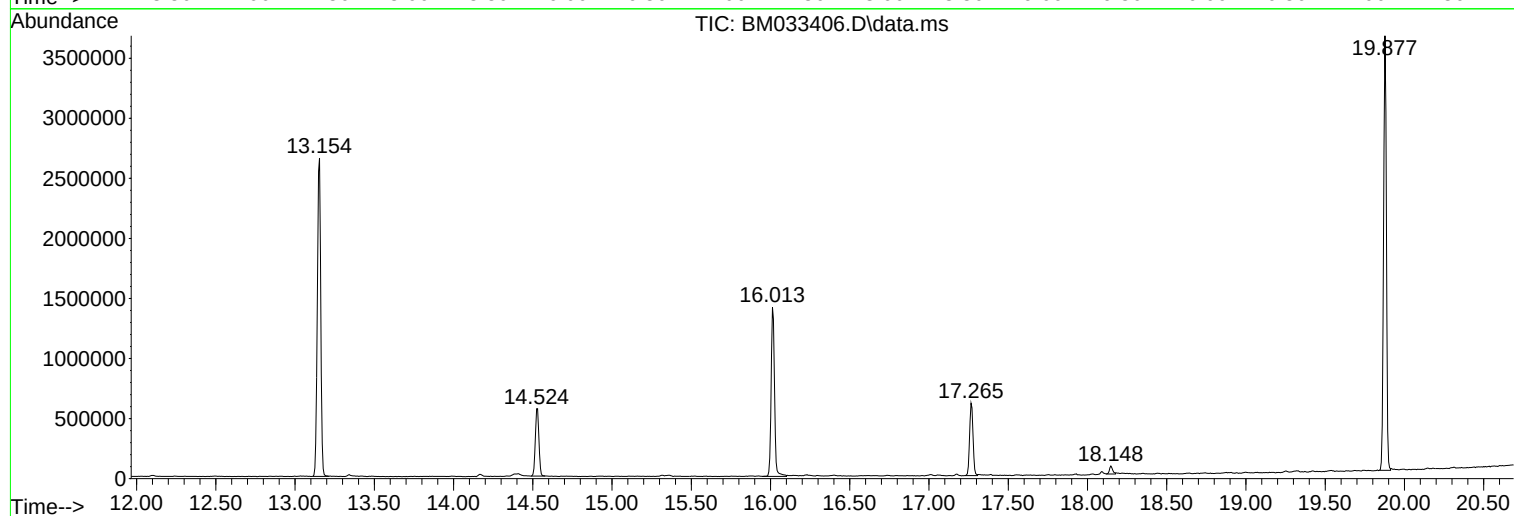
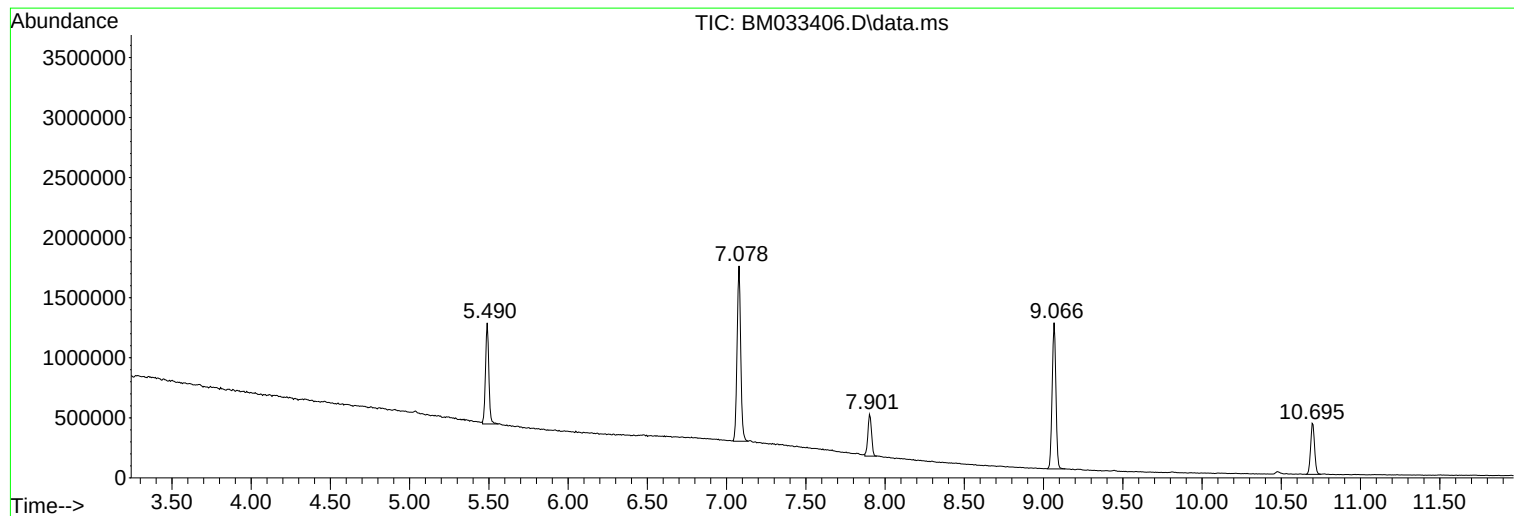
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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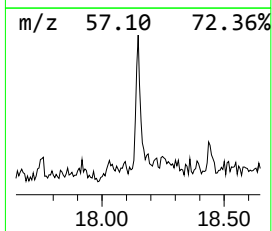
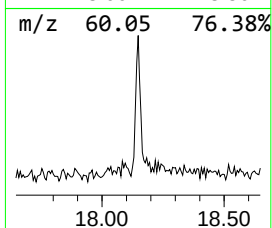
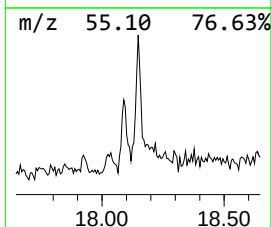
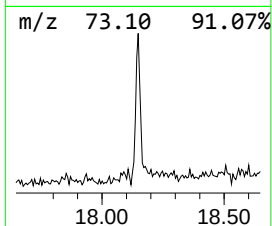
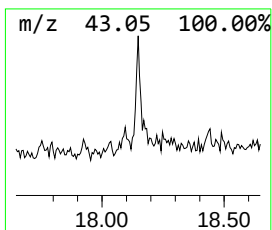
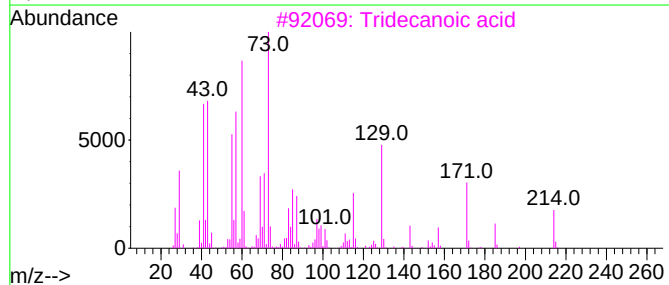
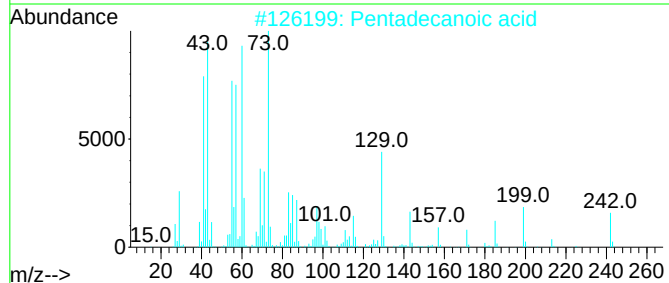
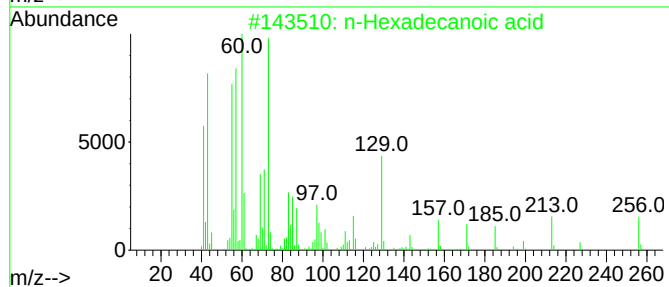
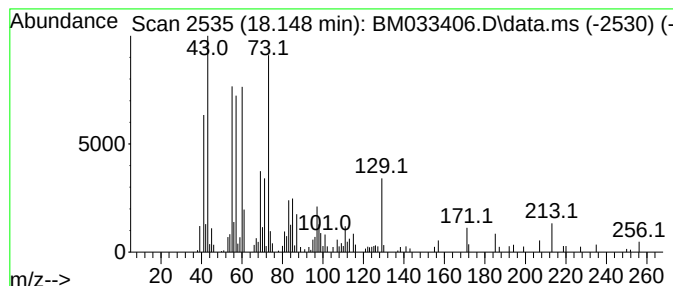
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.148	2.11 ng	94207	Phenanthrene-d10	17.265

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3		Tridecanoic acid	214	C13H26O2	000638-53-9	80
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	59
5		n-Decanoic acid	172	C10H20O2	000334-48-5	49



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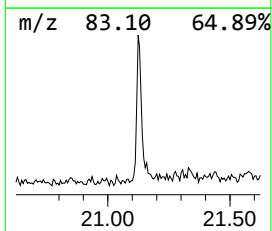
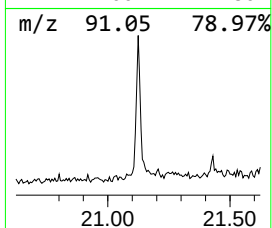
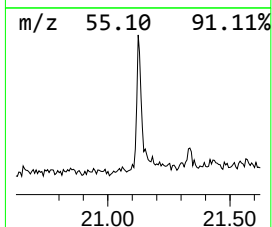
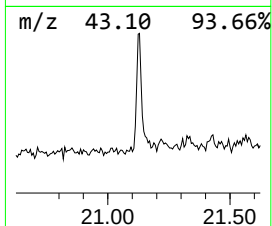
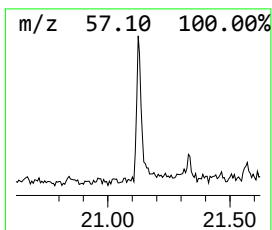
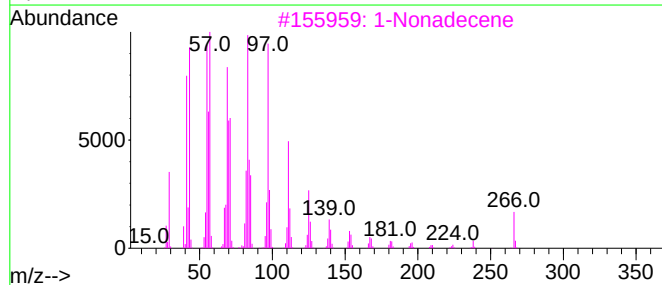
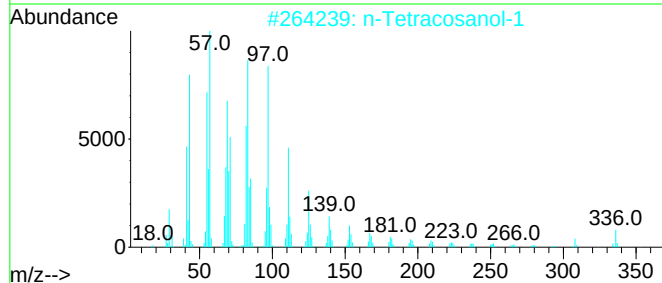
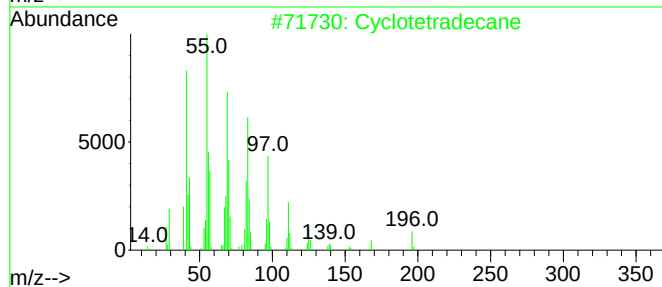
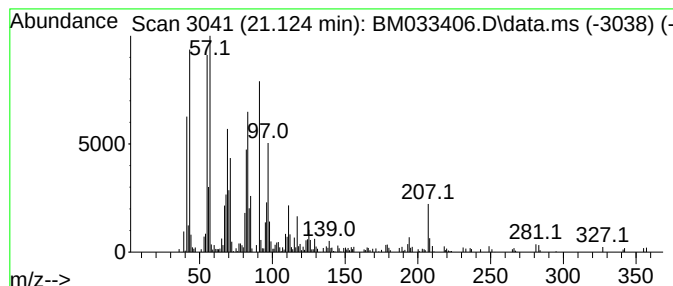
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Peak Number 2 Cyclotetradecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.124	4.83 ng	232346	Chrysene-d12	21.430

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclotetradecane	196	C14H28	000295-17-0	87
2			n-Tetracosanol-1	354	C24H50O	000506-51-4	87
3			1-Nonadecene	266	C19H38	018435-45-5	86
4			Octadecane, 1-(ethenyloxy)-	296	C20H40O	000930-02-9	83
5			17-Pentatriacontene	491	C35H70	006971-40-0	81



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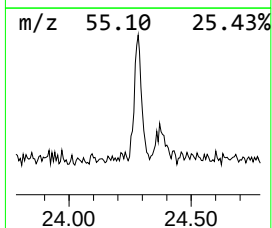
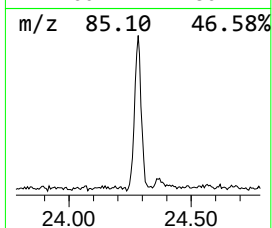
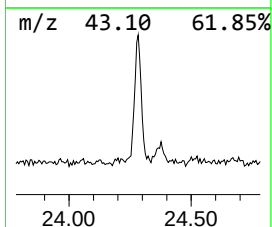
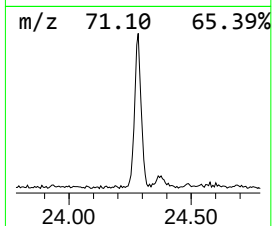
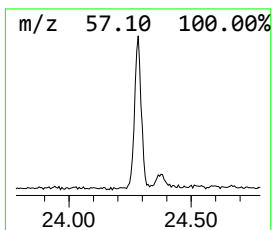
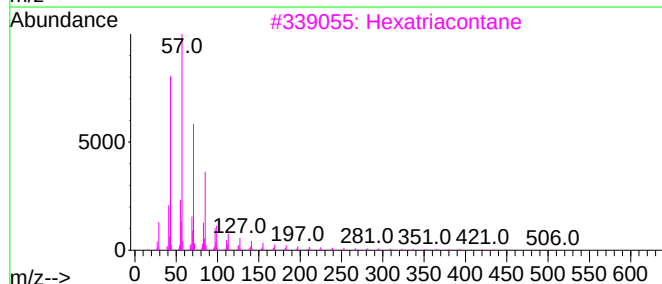
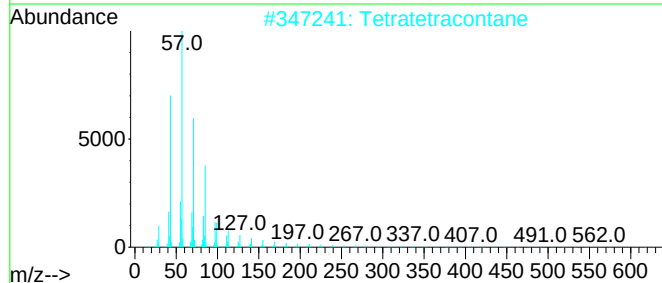
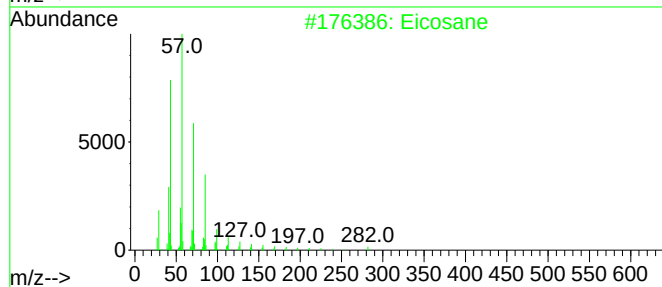
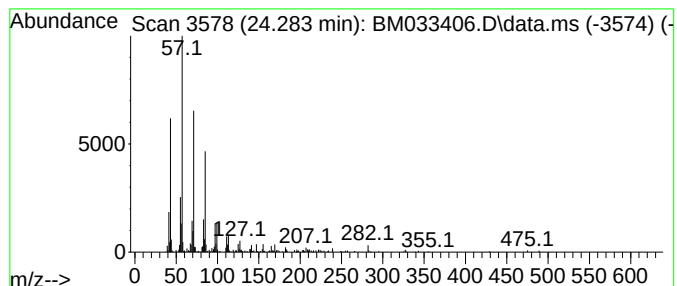
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Peak Number 3 Tetratetracontane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.283	6.86 ng	290318	Perylene-d12	23.747

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	91
2			Tetratetracontane	619	C44H90	007098-22-8	90
3			Hexatriacontane	507	C36H74	000630-06-8	87
4			Octacosane, 2-methyl-	408	C29H60	001560-98-1	87
5			Octacosane	394	C28H58	000630-02-4	87



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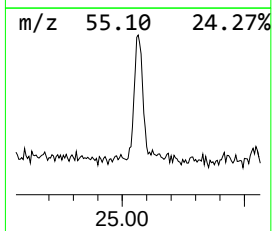
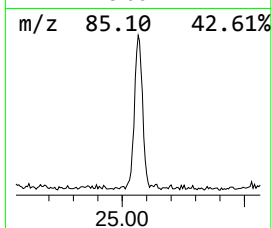
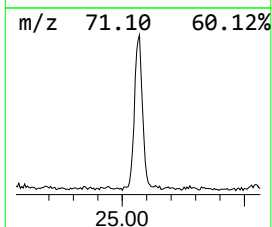
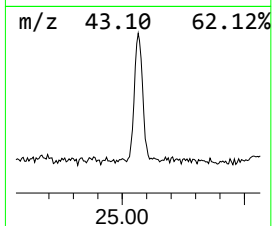
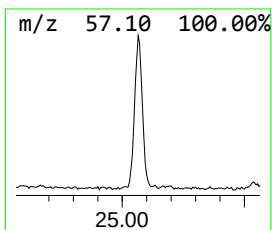
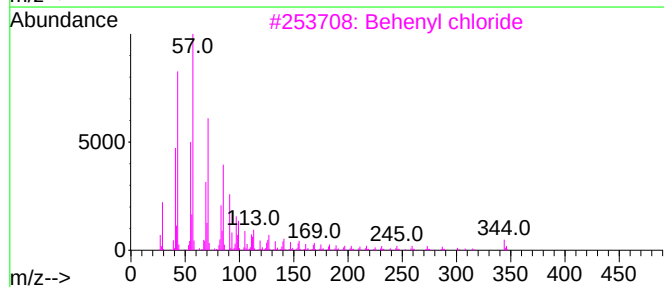
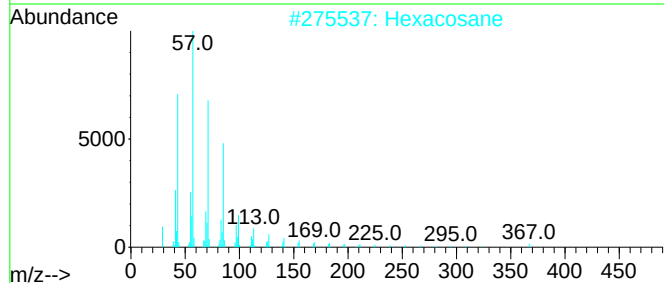
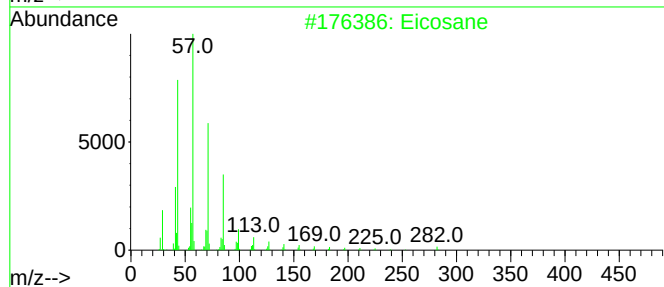
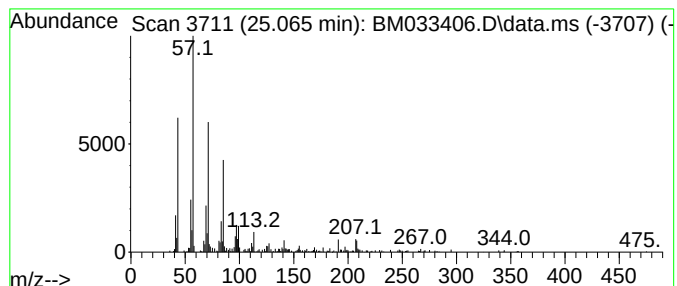
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Peak Number 4 Eicosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.065	7.80 ng	329960	Perylene-d12	23.747

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	94
2			Hexacosane	366	C26H54	000630-01-3	87
3			Behenyl chloride	344	C22H45Cl	042217-03-8	87
4			Octacosane	394	C28H58	000630-02-4	87
5			Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	87



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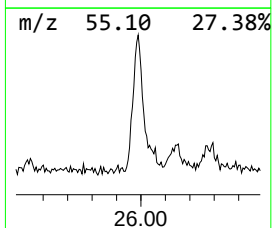
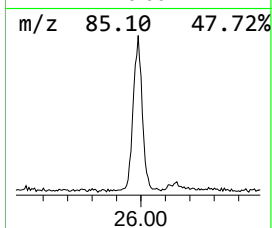
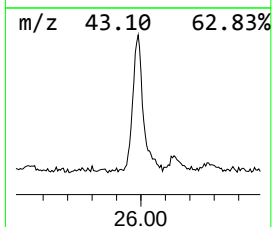
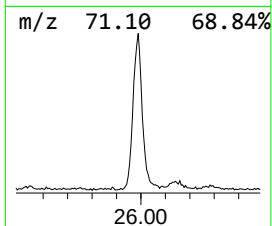
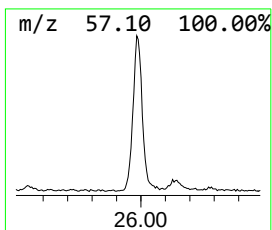
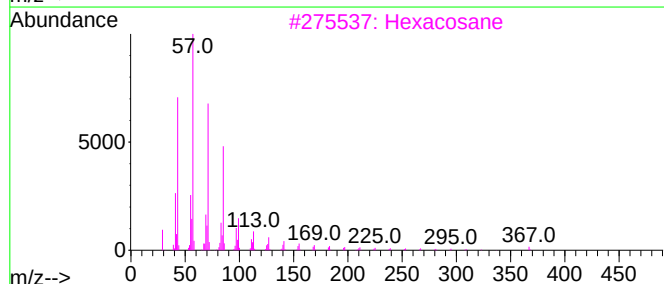
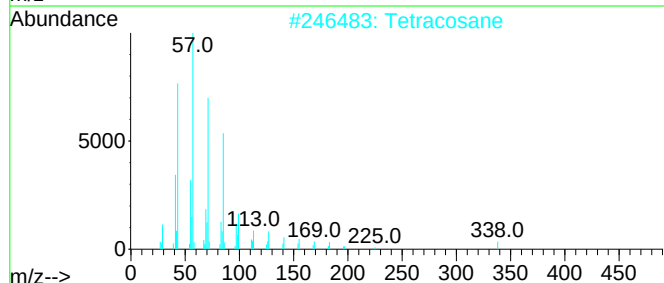
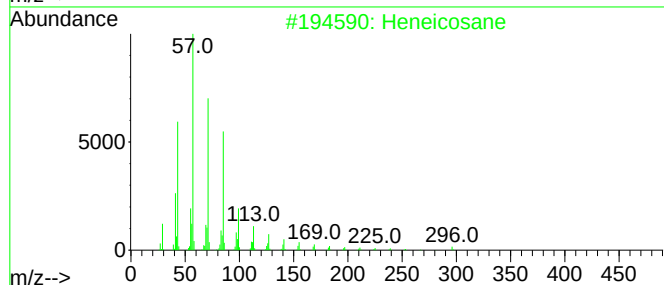
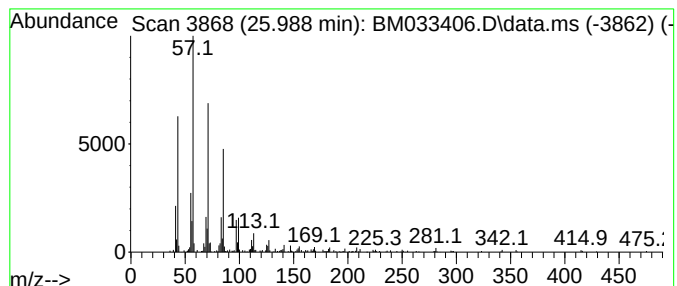
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Peak Number 5 Heneicosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.988	9.78 ng	413945	Perylene-d12	23.747

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	95
2			Tetracosane	338	C24H50	000646-31-1	90
3			Hexacosane	366	C26H54	000630-01-3	90
4			Octacosane	394	C28H58	000630-02-4	90
5			Tridecane, 6-propyl-	226	C16H34	055045-10-8	87



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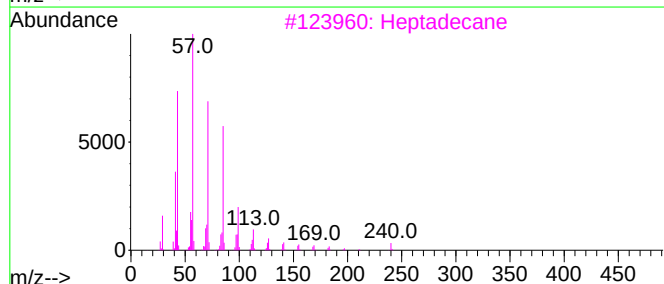
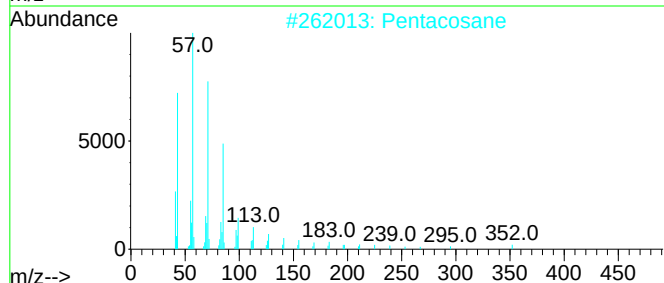
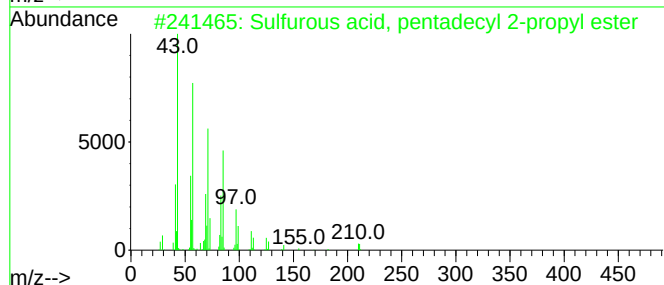
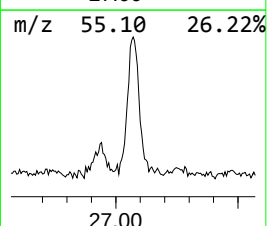
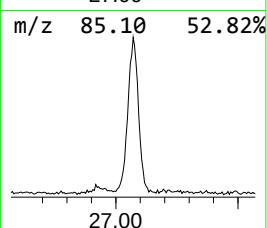
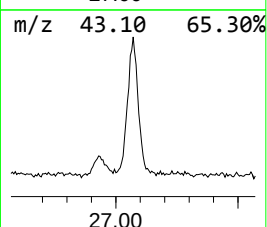
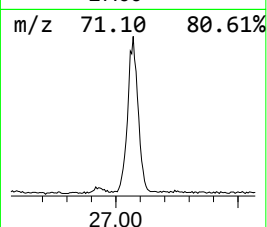
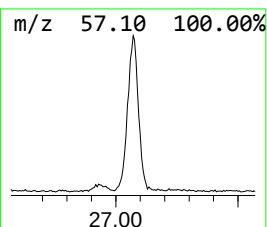
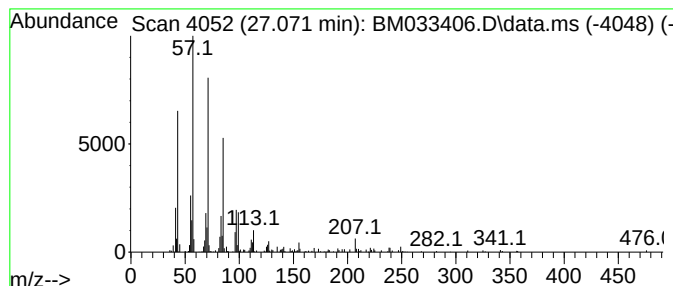
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Sulfurous acid, pentadecyl ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.071	14.51 ng	614210	Perylene-d12	23.747

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, pentadecyl 2-pro...	334	C18H38O3S	1000309-12-6	78
2			Pentacosane	352	C25H52	000629-99-2	74
3			Heptadecane	240	C17H36	000629-78-7	72
4			Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	72
5			Octacosane, 2-methyl-	408	C29H60	001560-98-1	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121021\
Data File : BM033406.D
Acq On : 10 Dec 2021 22:14
Operator : CG/JU
Sample : M4927-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PH1-BOT-6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM120821.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
n-Hexadecanoic ...	18.148	2.1	ng	94207	4	17.265	892915	20.0
Cyclotetradecane	21.124	4.8	ng	232346	5	21.430	961835	20.0
Tetratetracontane	24.283	6.9	ng	290318	6	23.747	846444	20.0
Eicosane	25.065	7.8	ng	329960	6	23.747	846444	20.0
Heneicosane	25.988	9.8	ng	413945	6	23.747	846444	20.0
Sulfurous acid,...	27.071	14.5	ng	614210	6	23.747	846444	20.0