

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052822\
 Data File : BM035308.D
 Acq On : 28 May 2022 14:11
 Operator : CG/JU
 Sample : N2933-23
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 P023-SS005-0006-01

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-BM052722.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM035308.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.457	396	403	418	rBV	1109284	1702148	48.59%	7.821%
2	7.046	666	673	691	rBV	1020760	1692029	48.30%	7.774%
3	7.875	807	814	824	rBV	362341	587306	16.77%	2.698%
4	9.034	1004	1011	1023	rBV	625370	1074405	30.67%	4.936%
5	10.669	1283	1289	1306	rBV	417768	738694	21.09%	3.394%
6	13.133	1702	1708	1721	rBV	1634011	2442482	69.73%	11.222%
7	14.510	1935	1942	1953	rBV	609692	895446	25.56%	4.114%
8	15.998	2188	2195	2213	rBV	1128658	1643022	46.91%	7.549%
9	17.257	2401	2409	2415	rBV	675030	1004452	28.68%	4.615%
10	18.157	2557	2562	2571	rBV	186635	276885	7.90%	1.272%
11	19.315	2756	2759	2767	rVB3	21601	35732	1.02%	0.164%
12	19.433	2775	2779	2790	rBV	108928	172294	4.92%	0.792%
13	19.786	2835	2839	2846	rBV	341017	427897	12.22%	1.966%
14	19.874	2849	2854	2861	rBV	2858186	3502836	100.00%	16.094%
15	21.156	3067	3072	3081	rVB2	280773	423247	12.08%	1.945%
16	21.351	3103	3105	3108	rVB	64540	60469	1.73%	0.278%
17	21.433	3114	3119	3128	rBV	1122144	1555491	44.41%	7.147%
18	23.086	3396	3400	3405	rVB	316071	450198	12.85%	2.068%
19	23.797	3515	3521	3531	rVB2	871140	1733097	49.48%	7.963%
20	24.409	3621	3625	3634	rVB	226082	449973	12.85%	2.067%
21	24.515	3637	3643	3658	rVB	326950	896420	25.59%	4.119%

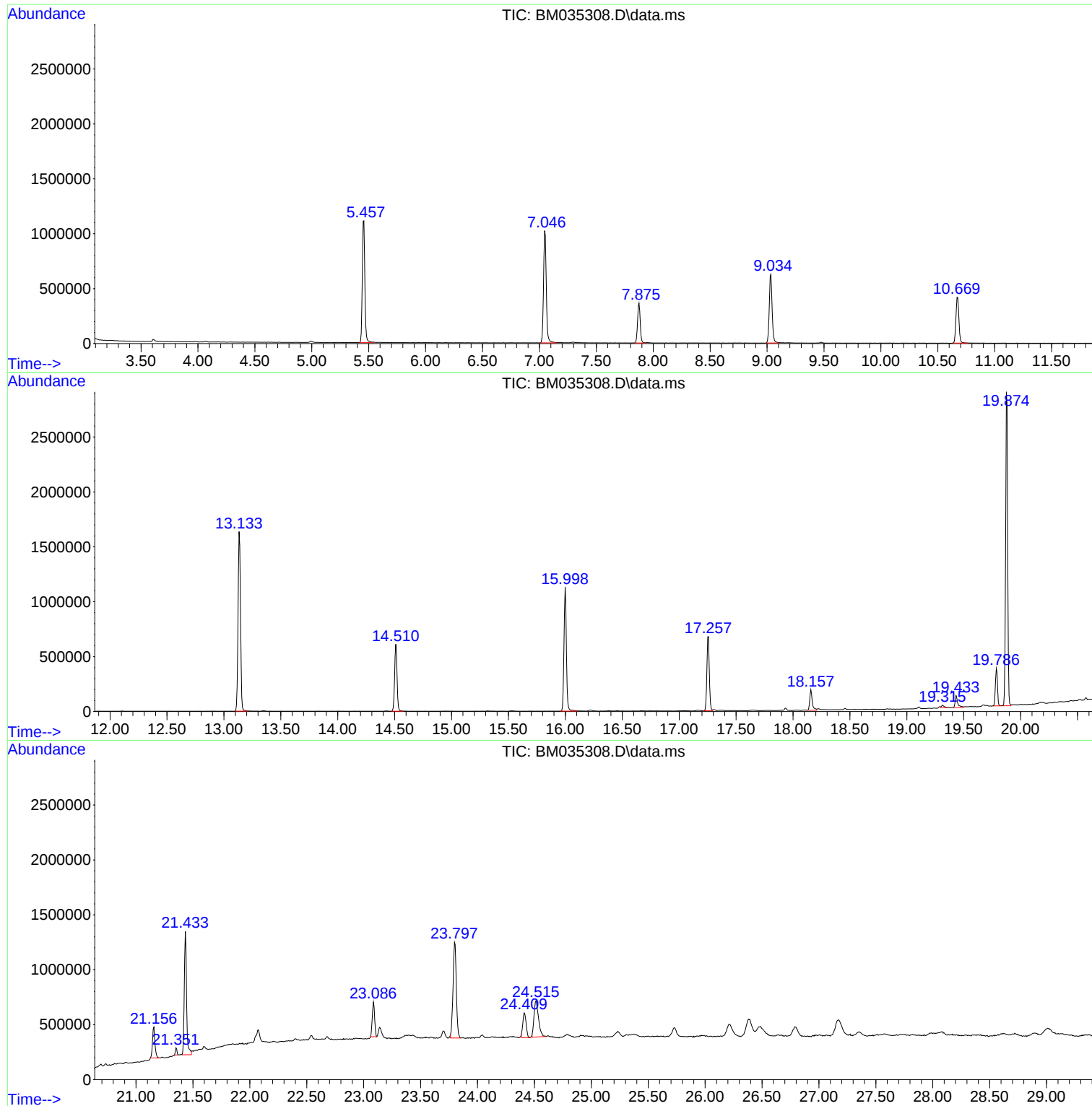
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM052722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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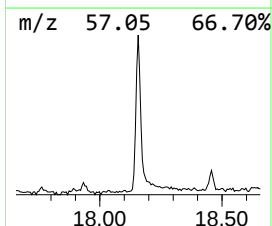
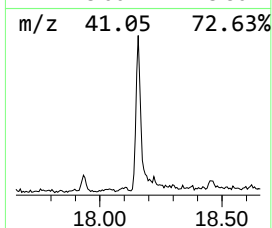
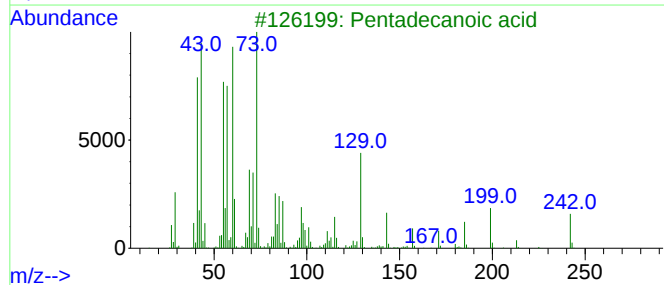
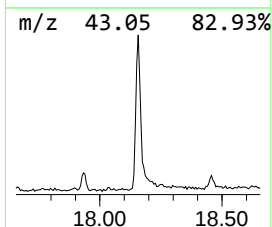
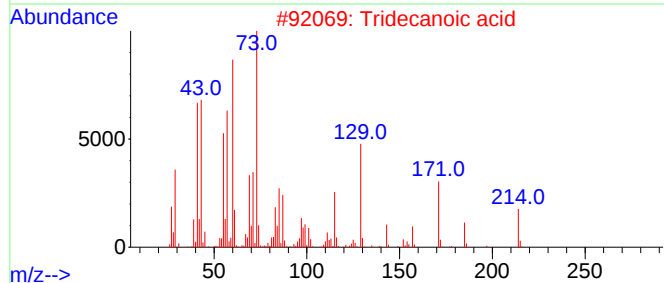
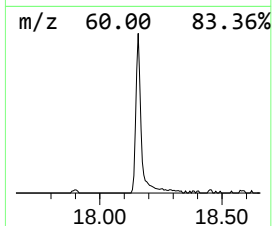
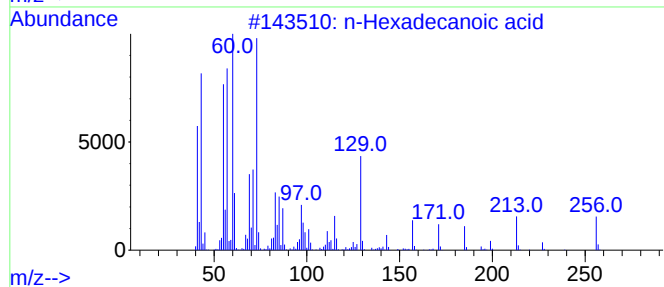
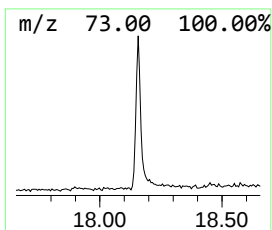
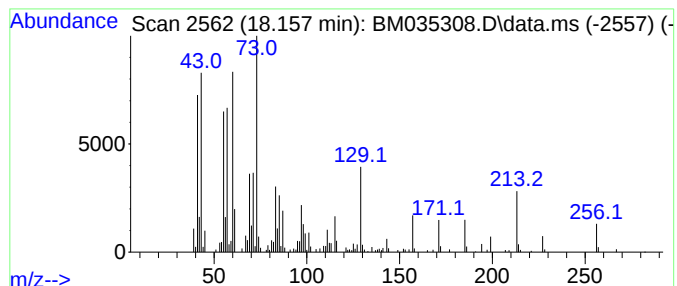
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.157	5.51 ng	276885	Phenanthrene-d10	17.257

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	97
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	86
5			n-Decanoic acid	172	C10H20O2	000334-48-5	58



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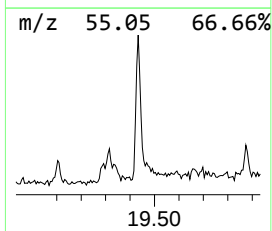
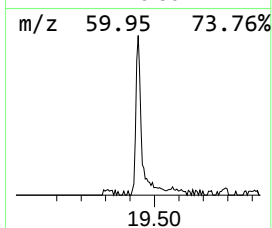
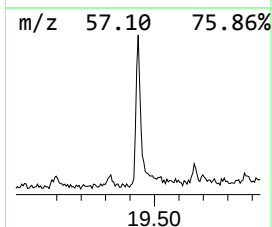
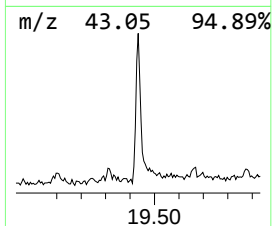
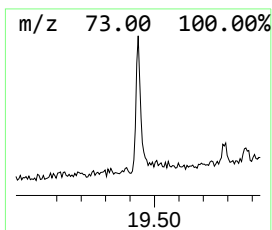
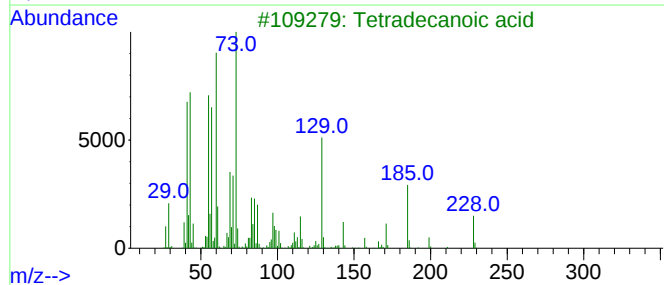
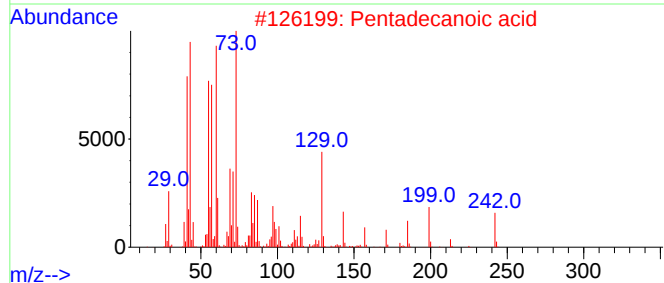
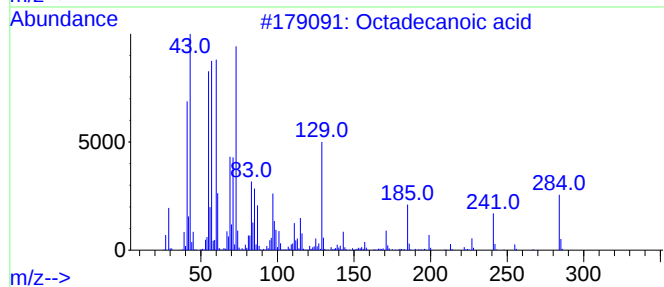
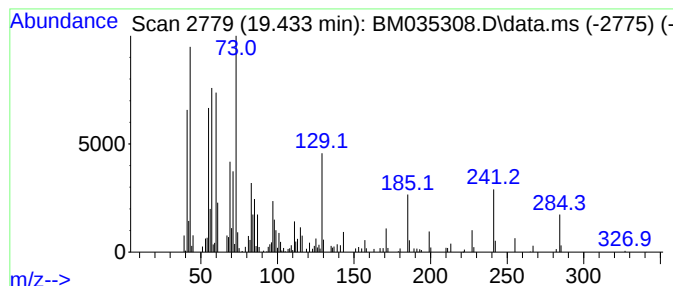
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.433	2.22 ng	172294	Chrysene-d12	21.433

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	81
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	76
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	68
5			n-Decanoic acid	172	C10H20O2	000334-48-5	60



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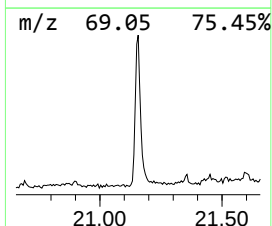
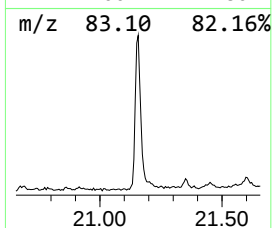
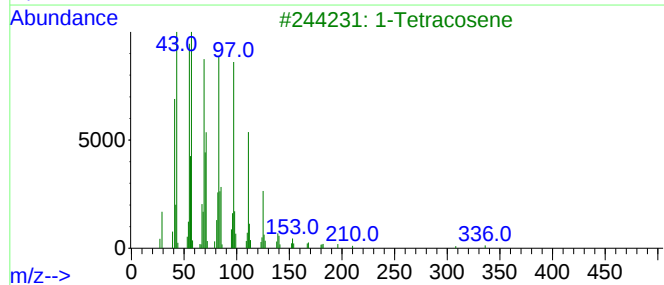
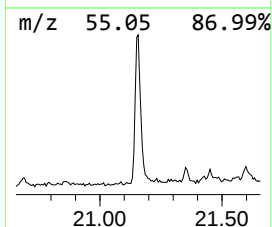
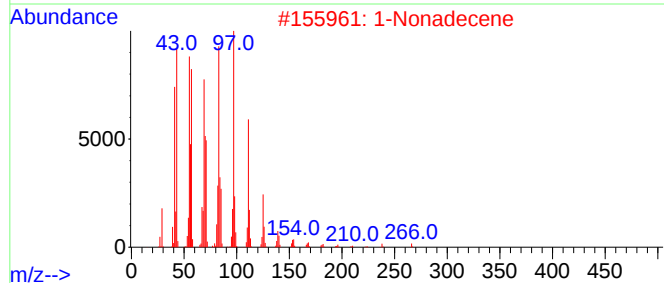
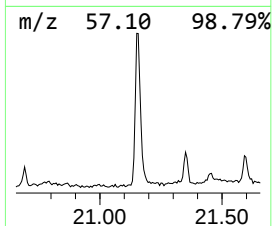
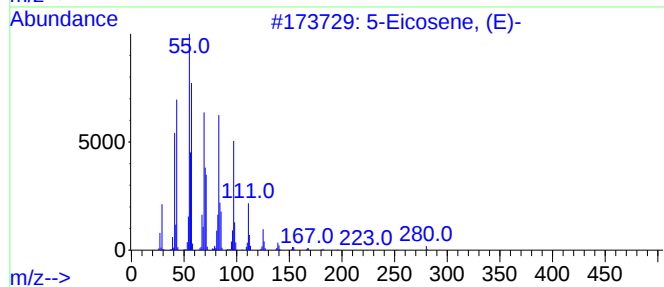
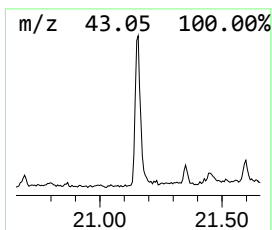
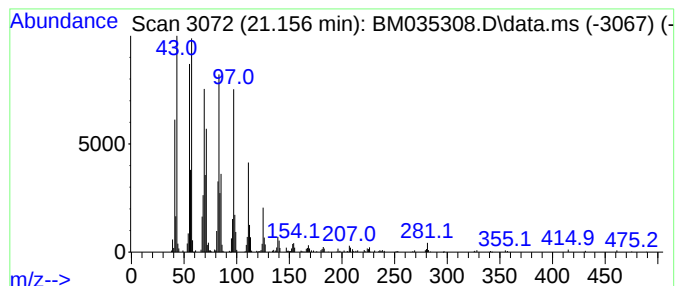
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Peak Number 4 5-Eicosene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.156	5.44 ng	423247	Chrysene-d12	21.433

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-		280	C20H40	074685-30-6	98
2	1-Nonadecene		266	C19H38	018435-45-5	96
3	1-Tetracosene		336	C24H48	010192-32-2	95
4	1-Hexacosene		364	C26H52	018835-33-1	95
5	Heptafluorobutyric acid, pentade...		424	C19H31F7O2	959261-23-5	94



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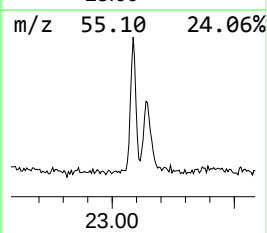
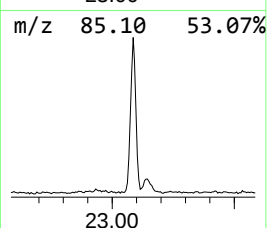
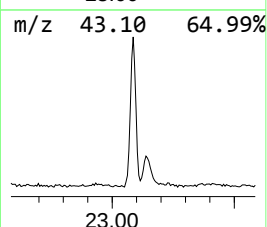
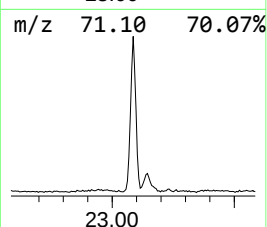
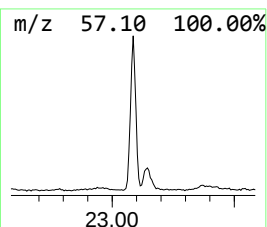
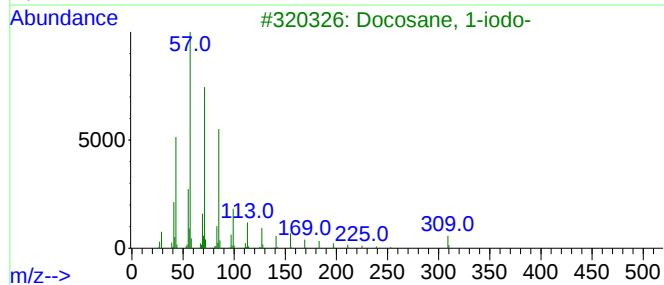
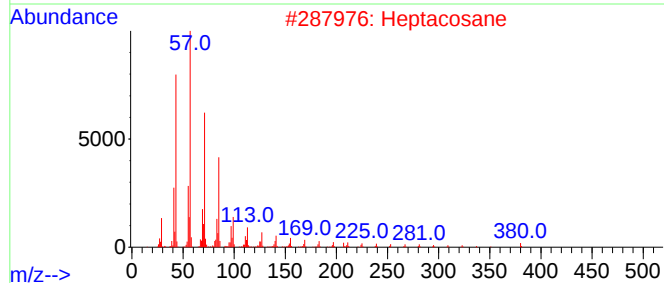
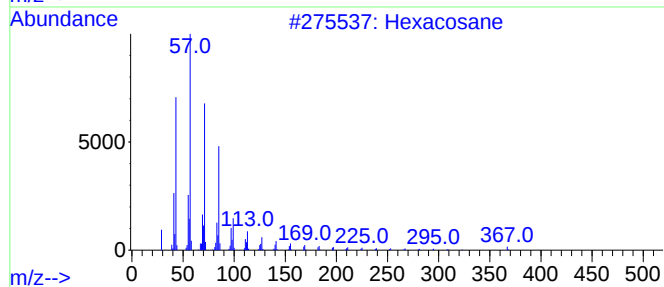
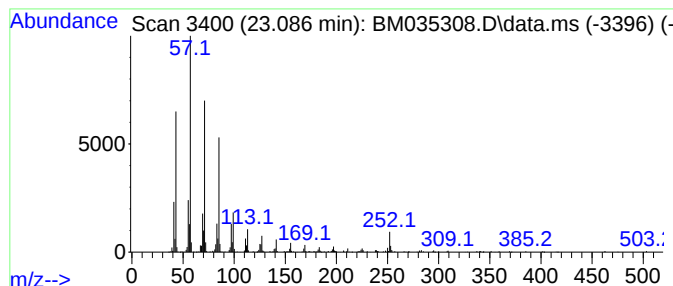
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Peak Number 5 Hexacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.086	5.20 ng	450198	Perylene-d12	23.797

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	93
2			Heptacosane	380	C27H56	000593-49-7	87
3			Docosane, 1-iodo-	436	C22H45I	1000406-31-9	87
4			Octacosane, 2-methyl-	408	C29H60	001560-98-1	87
5			Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	87



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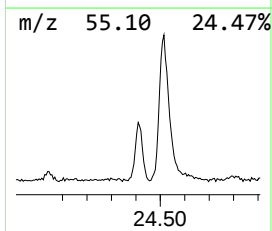
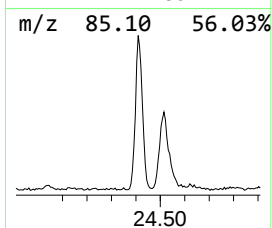
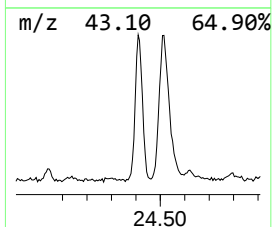
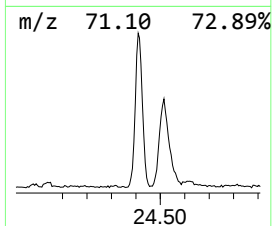
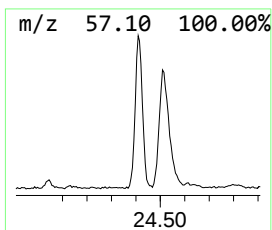
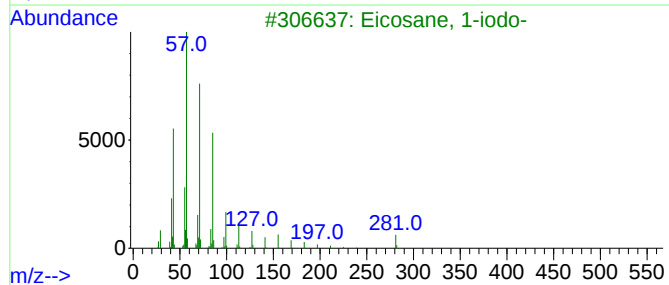
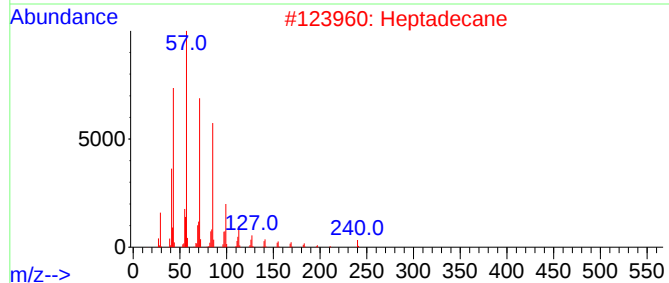
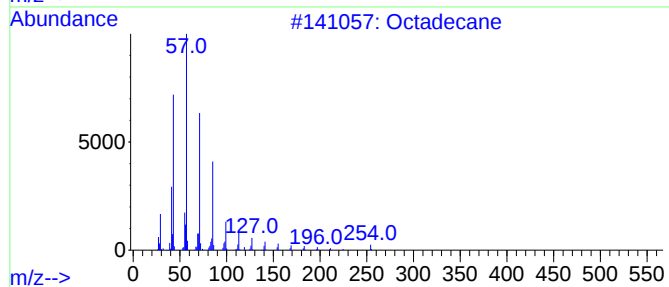
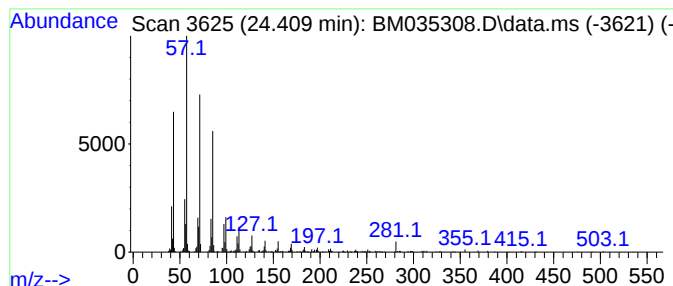
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TIC Library : C:\Database\NIST20.L
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Peak Number 6 Octadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.409	5.19 ng	449973	Perylene-d12	23.797

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecane	254	C18H38	000593-45-3	96
2			Heptadecane	240	C17H36	000629-78-7	91
3			Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	90
4			Octacosane, 2-methyl-	408	C29H60	001560-98-1	90
5			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90



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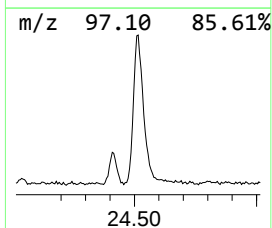
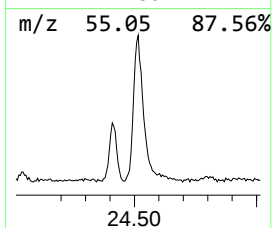
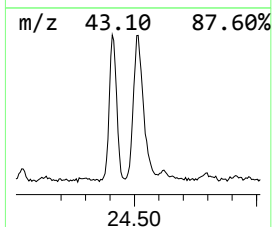
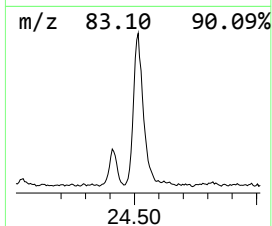
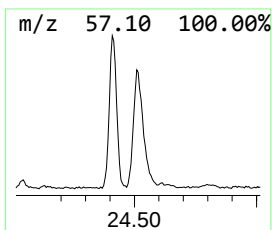
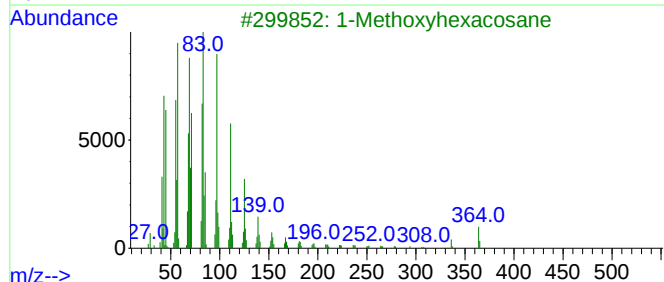
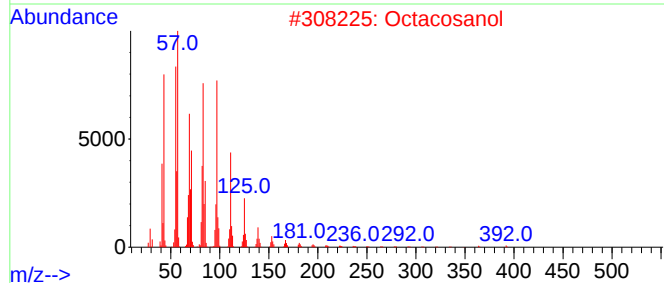
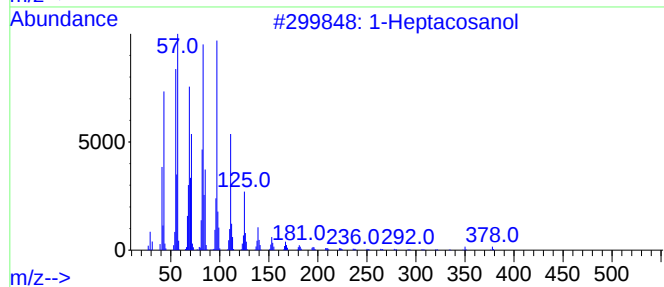
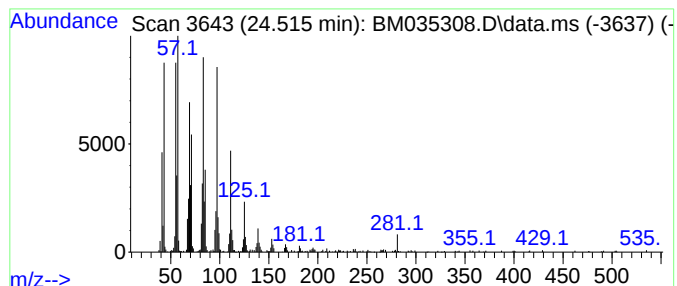
Instrument :
BNA_M
ClientSampleId :
P023-SS005-0006-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM052722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Heptacosanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD		R.T.	
24.515	10.34 ng	896420	Perylene-d12		23.797	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	1-Heptacosanol		396	C27H56O	002004-39-9	95
2	Octacosanol		410	C28H58O	000557-61-9	95
3	1-Methoxyhexacosane		396	C27H56O	237742-59-5	94
4	Heptadecyl heptafluorobutyrate		452	C21H35F7O2	959085-66-6	94
5	n-Tetracosanol-1		354	C24H50O	000506-51-4	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052822\
Data File : BM035308.D
Acq On : 28 May 2022 14:11
Operator : CG/JU
Sample : N2933-23
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P023-SS005-0006-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM052722.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 ...	18.157	5.5	ng	276885	4	17.257	1004450	20.0
Octadecanoic acid	19.433	2.2	ng	172294	5	21.433	1555490	20.0
5-Eicosene, (E)-	21.156	5.4	ng	423247	5	21.433	1555490	20.0
Hexacosane	23.086	5.2	ng	450198	6	23.797	1733100	20.0
Octadecane	24.409	5.2	ng	449973	6	23.797	1733100	20.0
1-Heptacosanol	24.515	10.3	ng	896420	6	23.797	1733100	20.0