

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM060122\
 Data File : BM035347.D
 Acq On : 01 Jun 2022 15:12
 Operator : CG/JU
 Sample : N3107-01
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 MS-5

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: BM035347.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.446	395	401	417	rBV	1872233	2824273	52.30%	6.062%
2	7.045	662	673	688	rBV	1795009	2870216	53.15%	6.161%
3	7.863	805	812	820	rBV	445326	712230	13.19%	1.529%
4	9.022	1002	1009	1020	rBV	1123713	1878044	34.78%	4.031%
5	10.663	1279	1288	1302	rBV	550836	958299	17.75%	2.057%
6	13.127	1700	1707	1724	rBV	3068956	4425693	81.96%	9.500%
7	14.210	1886	1891	1901	rVB2	68333	118248	2.19%	0.254%
8	14.498	1933	1940	1948	rBV	784534	1226062	22.71%	2.632%
9	15.992	2187	2194	2217	rBV	2253420	3275277	60.66%	7.030%
10	16.221	2228	2233	2242	rBV6	24596	60948	1.13%	0.131%
11	17.245	2401	2407	2411	rBV	971639	1371379	25.40%	2.944%
12	17.286	2411	2414	2420	rVB	291416	445615	8.25%	0.957%
13	17.380	2426	2430	2435	rVB	102846	149707	2.77%	0.321%
14	17.621	2466	2471	2475	rBV6	30908	60691	1.12%	0.130%
15	18.151	2553	2561	2574	rBV2	476652	828609	15.35%	1.779%
16	18.321	2585	2590	2594	rBV2	85774	145402	2.69%	0.312%
17	19.180	2732	2736	2743	rBV6	33582	71506	1.32%	0.153%
18	19.303	2752	2757	2763	rBV	723641	971750	18.00%	2.086%
19	19.362	2764	2767	2771	rVB2	98296	123962	2.30%	0.266%
20	19.427	2774	2778	2787	rVV2	246499	379113	7.02%	0.814%
21	19.668	2810	2819	2828	rBV	643533	1074421	19.90%	2.306%
22	19.874	2848	2854	2859	rBV	4415694	5399778	100.00%	11.591%
23	20.162	2900	2903	2906	rBV	121737	138445	2.56%	0.297%
24	20.268	2917	2921	2925	rBV	88606	116677	2.16%	0.250%
25	21.150	3067	3071	3078	rVB3	513048	650492	12.05%	1.396%
26	21.350	3101	3105	3109	rBV	375695	396712	7.35%	0.852%
27	21.433	3112	3119	3122	rBV2	1344179	2272126	42.08%	4.877%
28	22.044	3220	3223	3234	rVB2	609284	1350329	25.01%	2.898%
29	23.086	3394	3400	3405	rBV	2850458	4591760	85.04%	9.856%
30	23.133	3405	3408	3417	rVB2	481708	759085	14.06%	1.629%
31	23.691	3500	3503	3511	rVB2	362341	671923	12.44%	1.442%
32	23.797	3516	3521	3528	rVB2	833464	1565292	28.99%	3.360%
33	24.409	3618	3625	3634	rVB	2275383	4703765	87.11%	10.097%

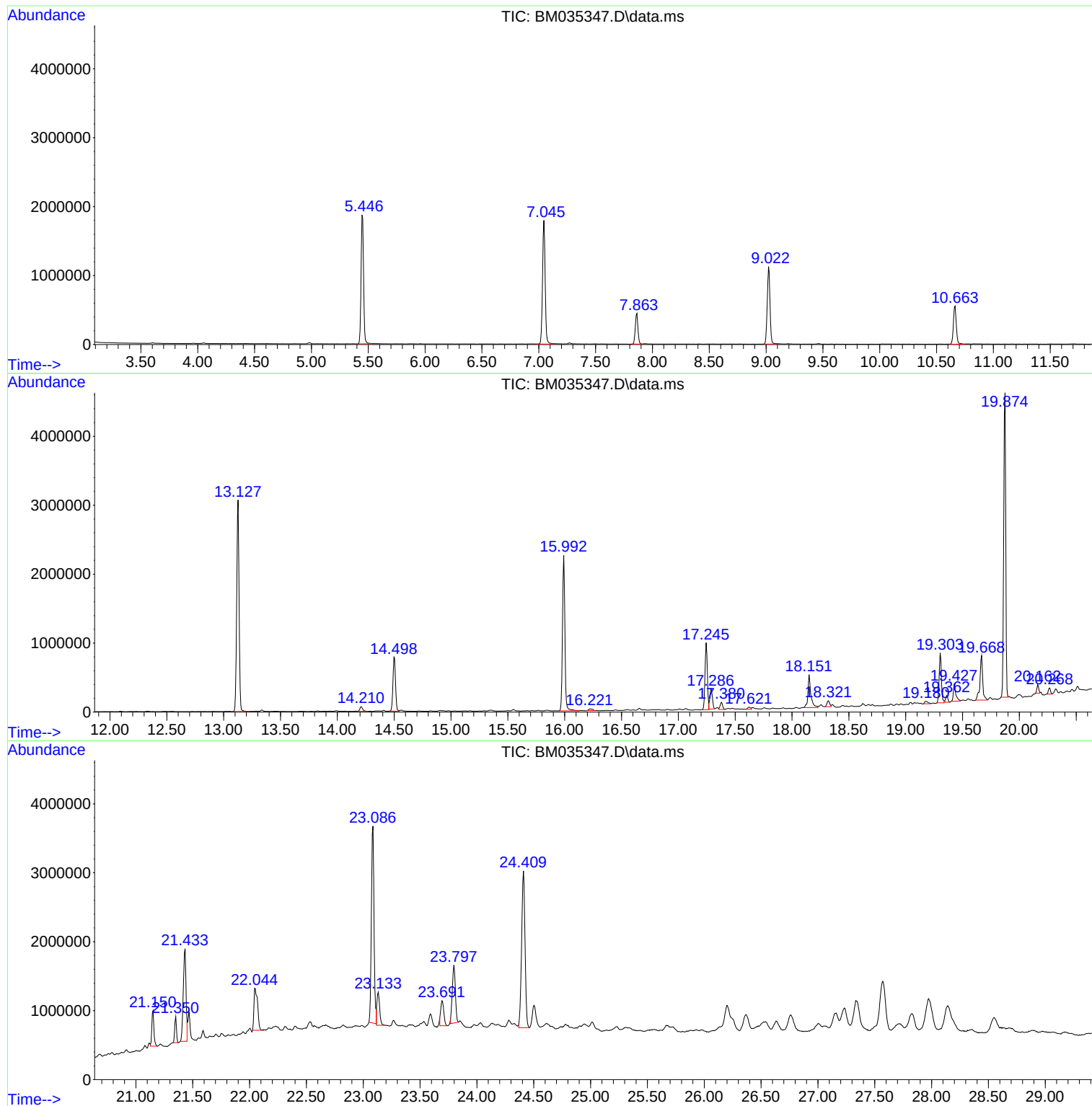
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM052722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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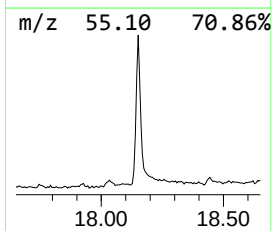
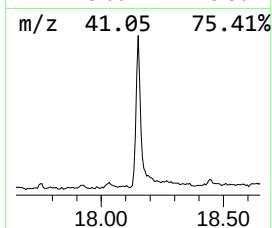
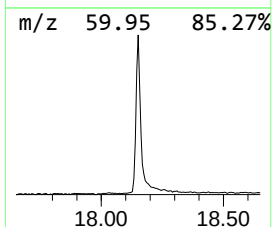
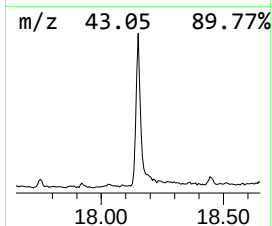
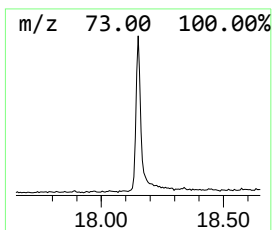
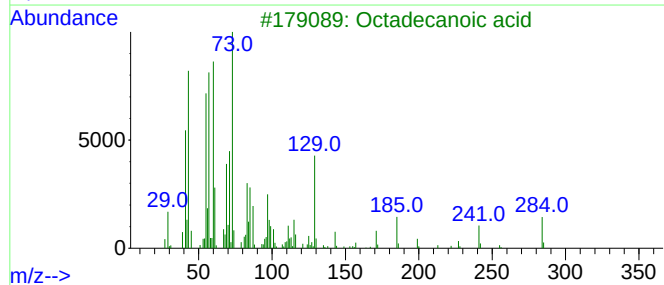
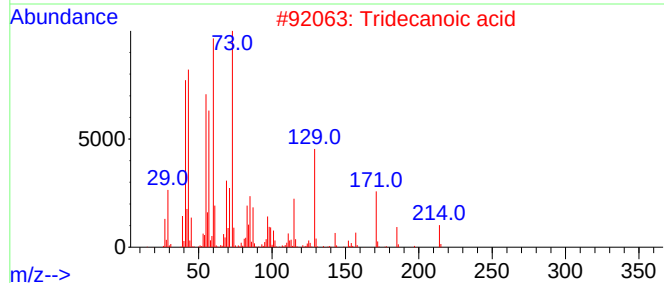
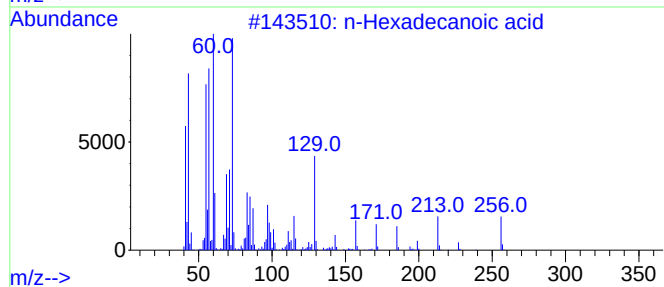
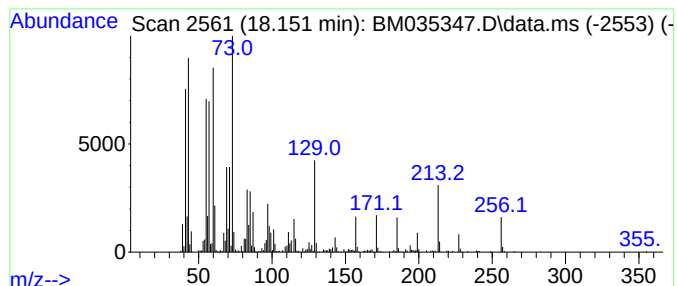
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.151	12.08 ng	828609	Phenanthrene-d10	17.245

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	89
3			Octadecanoic acid	284	C18H36O2	000057-11-4	87
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5			n-Decanoic acid	172	C10H20O2	000334-48-5	76



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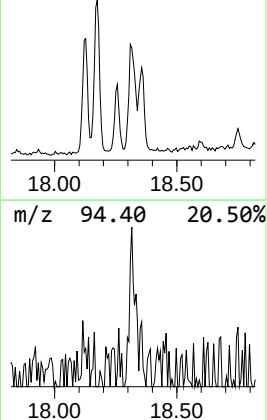
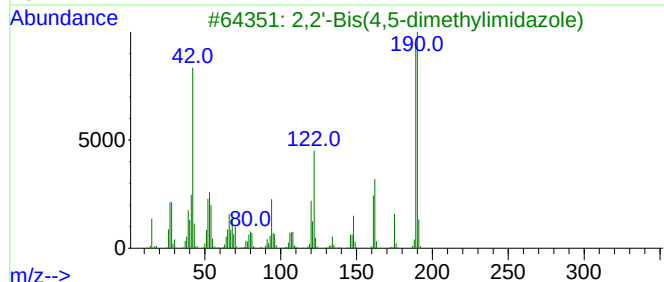
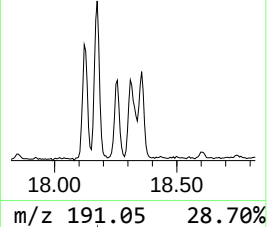
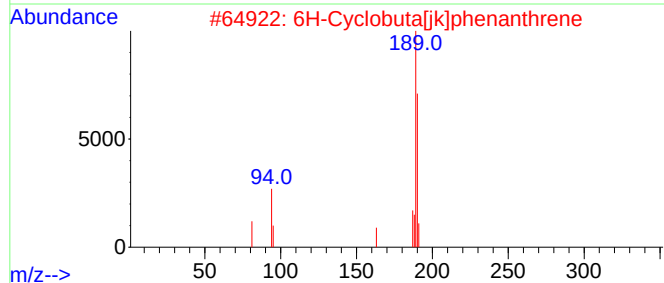
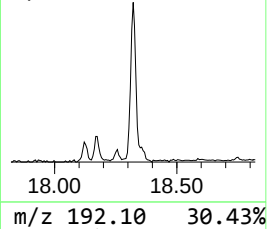
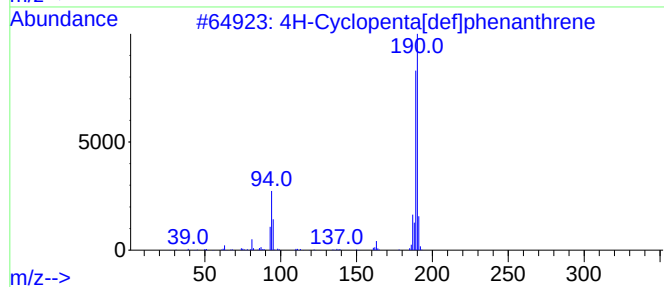
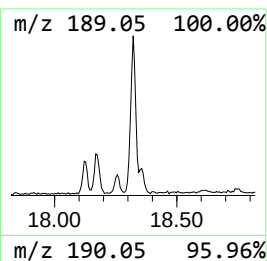
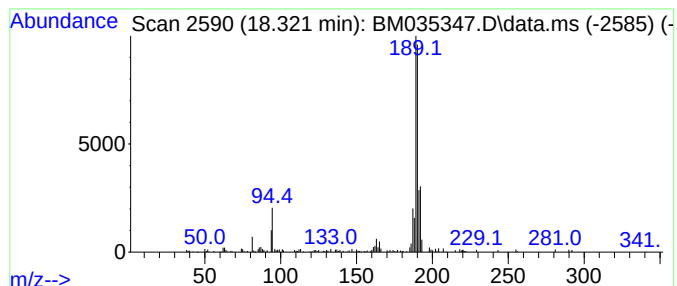
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM052722.M
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 4H-Cyclopenta[def]phenanthrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.321	2.12 ng	145402	Phenanthrene-d10	17.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	87
2			6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	72
3			2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	45
4			1,1'-Biphenyl, 4,4'-difluoro-	190	C12H8F2	000398-23-2	23
5			5-Bromo-4-fluoropyridin-2-amine	190	C5H4BrFN2	944401-69-8	18



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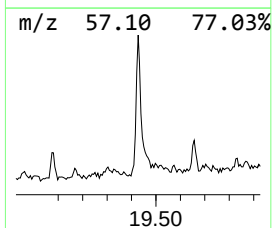
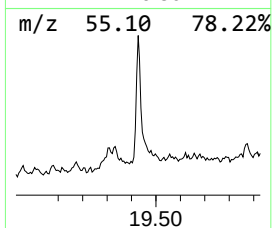
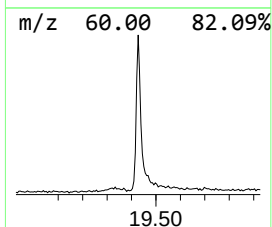
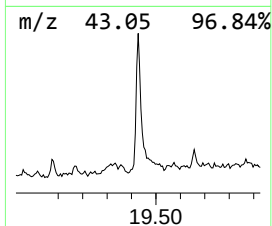
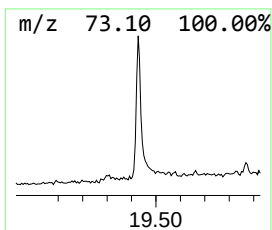
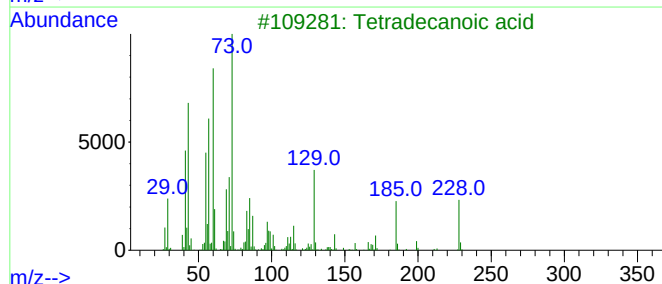
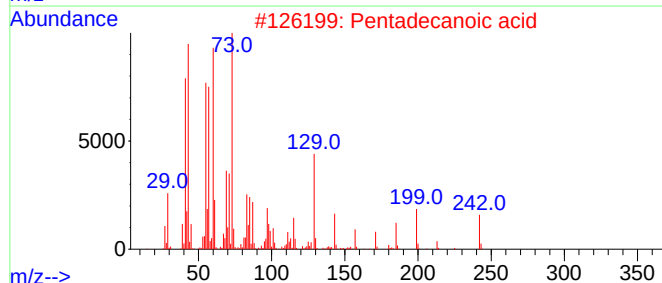
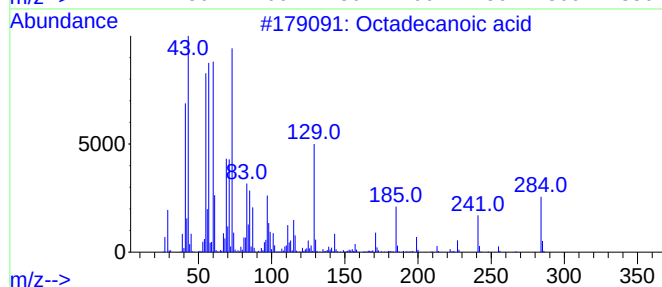
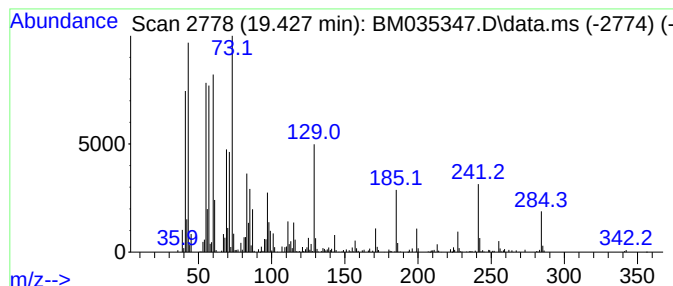
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.427	3.34 ng	379113	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	89
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	72
5			n-Decanoic acid	172	C10H20O2	000334-48-5	70



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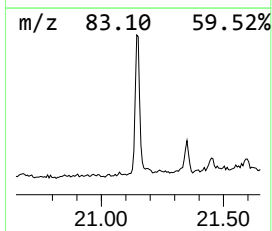
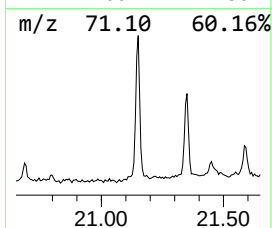
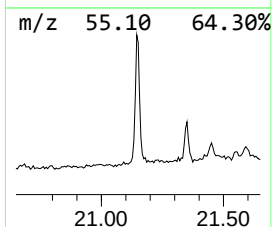
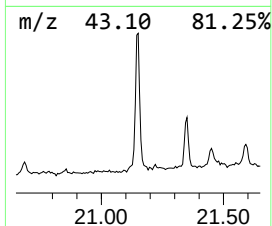
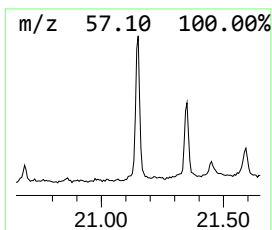
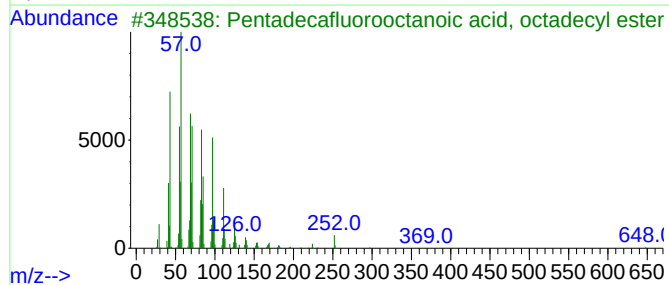
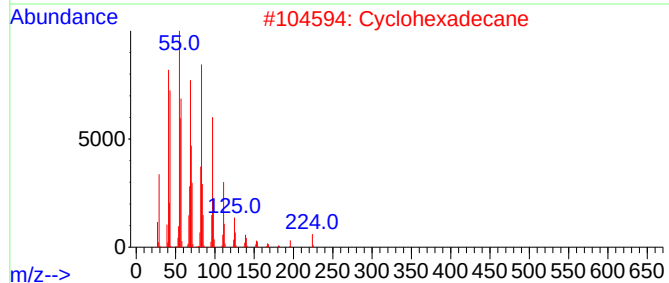
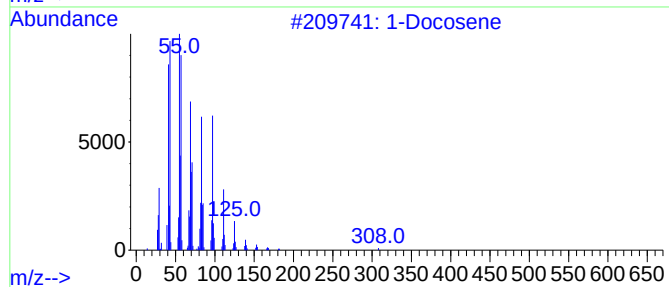
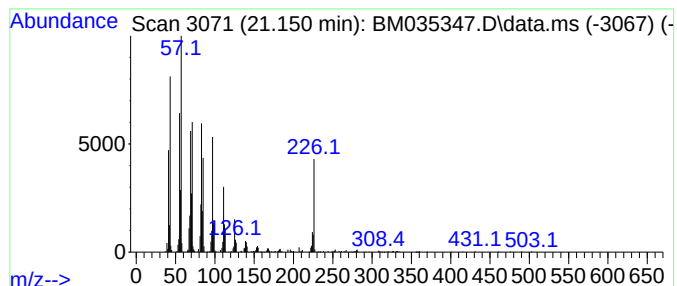
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 1-Docosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.150	5.73 ng	650492	Chrysene-d12	21.433

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene			308	C22H44	001599-67-3	93
2	Cyclohexadecane			224	C16H32	000295-65-8	90
3	Pentadecafluorooctanoic acid, oc...			666	C26H37F15O2	1000406-04-8	89
4	Pentadecafluorooctanoic acid, he...			638	C24H33F15O2	1000406-04-6	86
5	Oxalic acid, isobutyl octadecyl ...			398	C24H46O4	1000309-38-3	81



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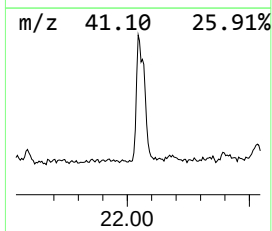
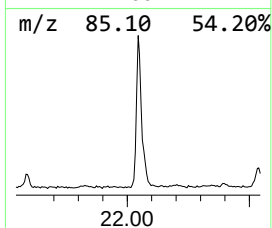
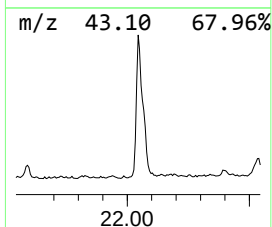
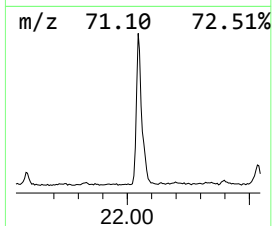
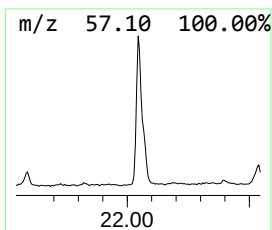
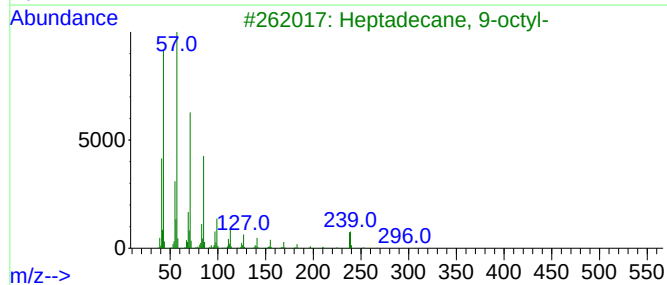
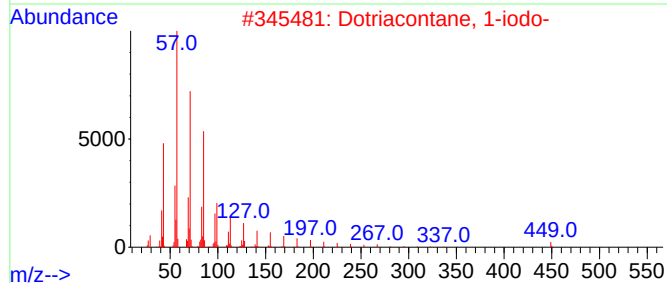
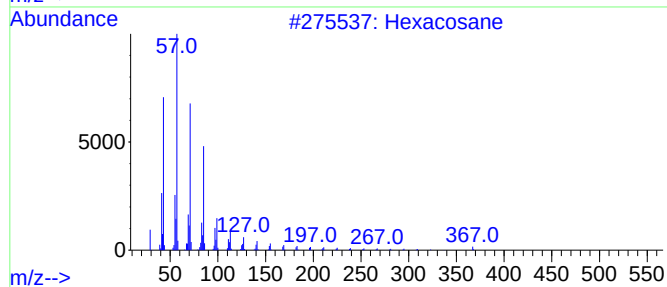
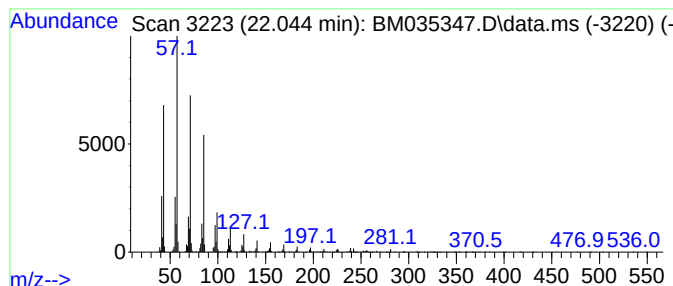
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Hexacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.044	11.89 ng	1350330	Chrysene-d12	21.433

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	93
2			Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	91
3			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4			Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
5			Octadecane	254	C18H38	000593-45-3	90



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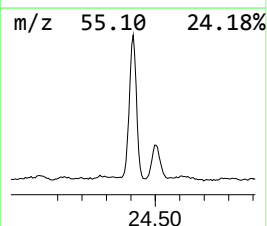
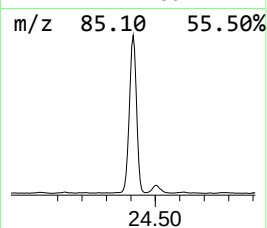
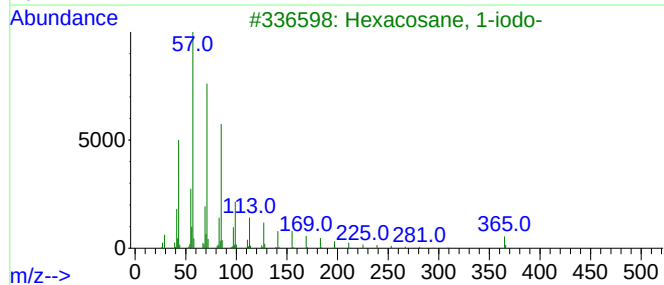
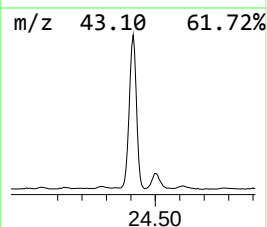
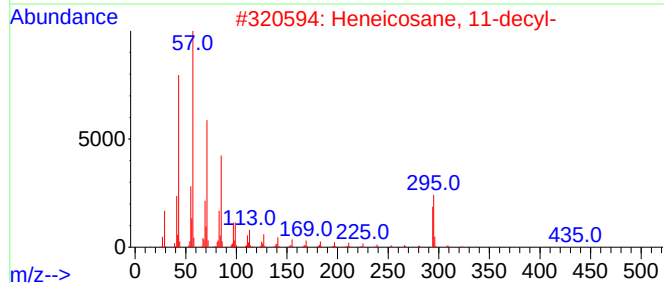
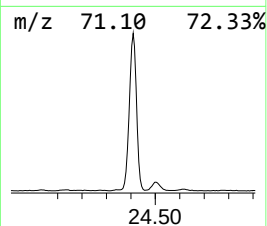
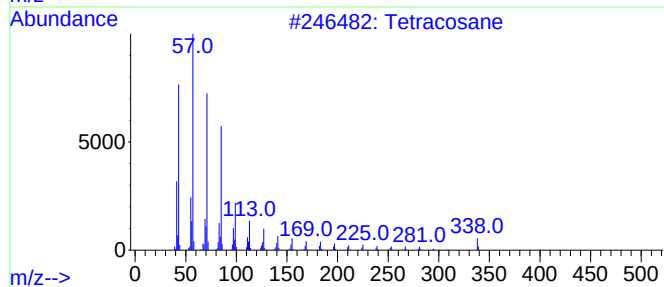
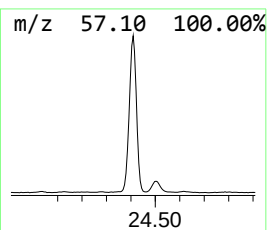
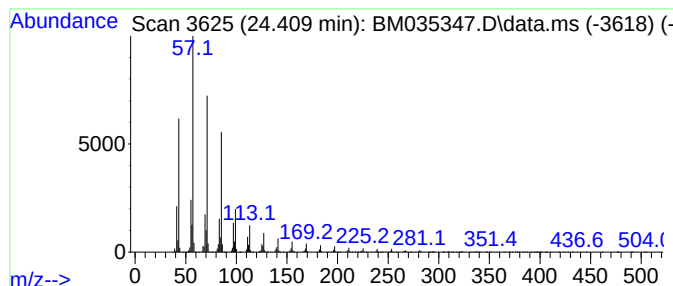
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM052722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Tetracosane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.409	60.10 ng	4703770	Perylene-d12	23.797

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracosane	338	C24H50	000646-31-1	98
2			Heneicosane, 11-decyl-	437	C31H64	055320-06-4	97
3			Hexacosane, 1-iodo-	492	C26H53I	1000406-32-1	91
4			Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	91
5			Triacontane	422	C30H62	000638-68-6	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM060122\
Data File : BM035347.D
Acq On : 01 Jun 2022 15:12
Operator : CG/JU
Sample : N3107-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MS-5

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Hexadecanoic ...	18.151	12.1	ng	828609	4	17.245	1371380	20.0
4H-Cyclopenta[d]...	18.321	2.1	ng	145402	4	17.245	1371380	20.0
Octadecanoic acid	19.427	3.3	ng	379113	5	21.433	2272130	20.0
1-Docosene	21.150	5.7	ng	650492	5	21.433	2272130	20.0
Hexacosane	22.044	11.9	ng	1350330	5	21.433	2272130	20.0
Tetracosane	24.409	60.1	ng	4703770	6	23.797	1565290	20.0