

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122623\
 Data File : BF136734.D
 Acq On : 26 Dec 2023 23:07
 Operator : CG\JU
 Sample : 05538-03
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 HR-03-112223

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_F\Methods\8270-BF122023.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136734.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.022	495	499	506	rBV	23378	28169	1.68%	0.237%
2	5.428	563	568	571	rBV	1528585	1432861	85.36%	12.048%
3	6.428	734	738	741	rBV	1462508	1436732	85.59%	12.080%
4	6.781	795	798	802	rBV	554939	438957	26.15%	3.691%
5	7.345	889	894	897	rBV	1091615	932353	55.54%	7.839%
6	8.057	1011	1015	1019	rBV	656773	547271	32.60%	4.602%
7	9.139	1194	1199	1202	rBV	1904512	1678614	100.00%	14.114%
8	9.251	1215	1218	1226	rVB	45493	48173	2.87%	0.405%
9	9.816	1310	1314	1317	rBV	674456	533409	31.78%	4.485%
10	10.610	1445	1449	1462	rBV	744133	701464	41.79%	5.898%
11	11.304	1564	1567	1571	rBV	532423	451569	26.90%	3.797%
12	11.580	1606	1614	1616	rBV5	11577	22834	1.36%	0.192%
13	11.839	1655	1658	1663	rBV	126115	118173	7.04%	0.994%
14	12.092	1698	1701	1704	rBV	43201	31856	1.90%	0.268%
15	12.392	1749	1752	1754	rBV2	19224	18242	1.09%	0.153%
16	12.557	1775	1780	1786	rBV7	9602	22037	1.31%	0.185%
17	12.627	1789	1792	1803	rVV	40545	56603	3.37%	0.476%
18	12.904	1834	1839	1842	rBV	1375119	1218970	72.62%	10.249%
19	13.339	1905	1913	1917	rBV3	35308	108721	6.48%	0.914%
20	13.857	1995	2001	2002	rBV5	36734	68972	4.11%	0.580%
21	13.962	2004	2019	2021	rBV	616040	1049320	62.51%	8.823%
22	14.004	2021	2026	2027	rBV2	171626	254331	15.15%	2.138%
23	14.304	2065	2077	2079	rBV2	86007	240045	14.30%	2.018%
24	14.821	2161	2165	2169	rBV	61017	64572	3.85%	0.543%
25	15.439	2265	2270	2274	rBV	287942	388900	23.17%	3.270%

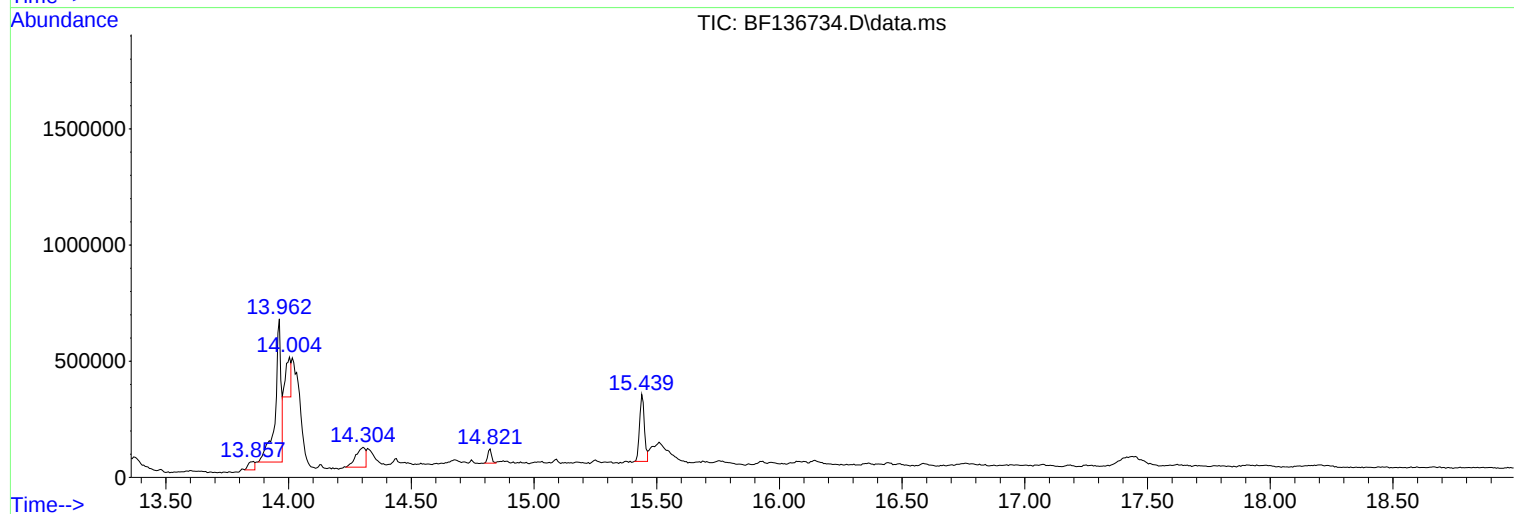
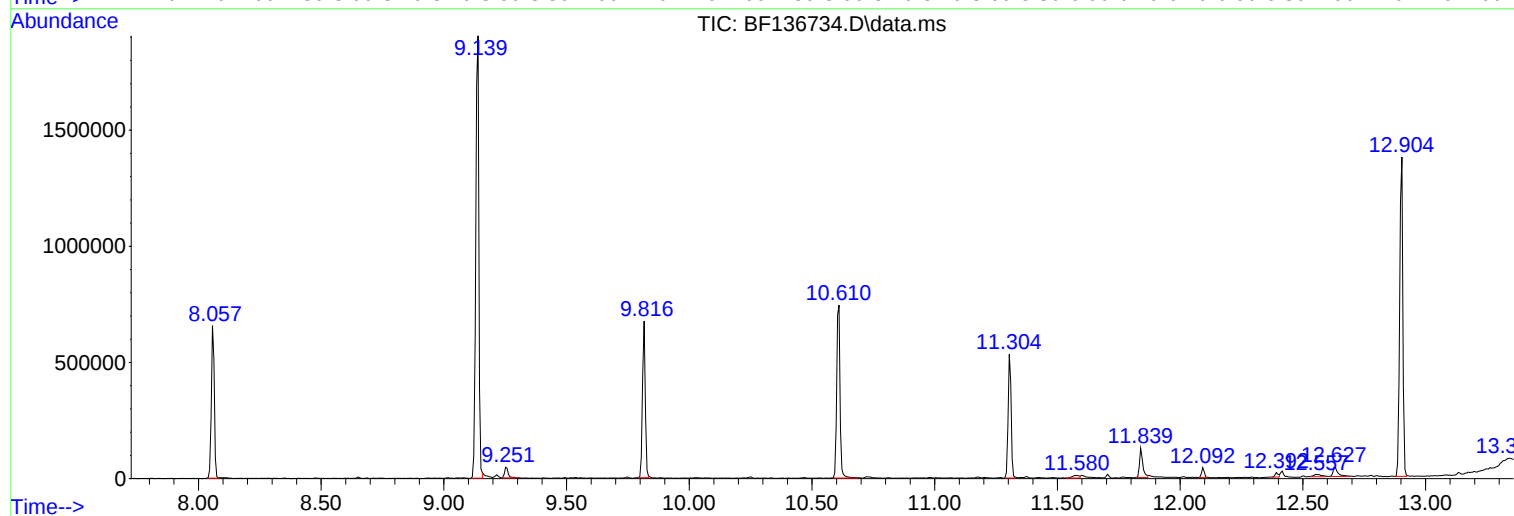
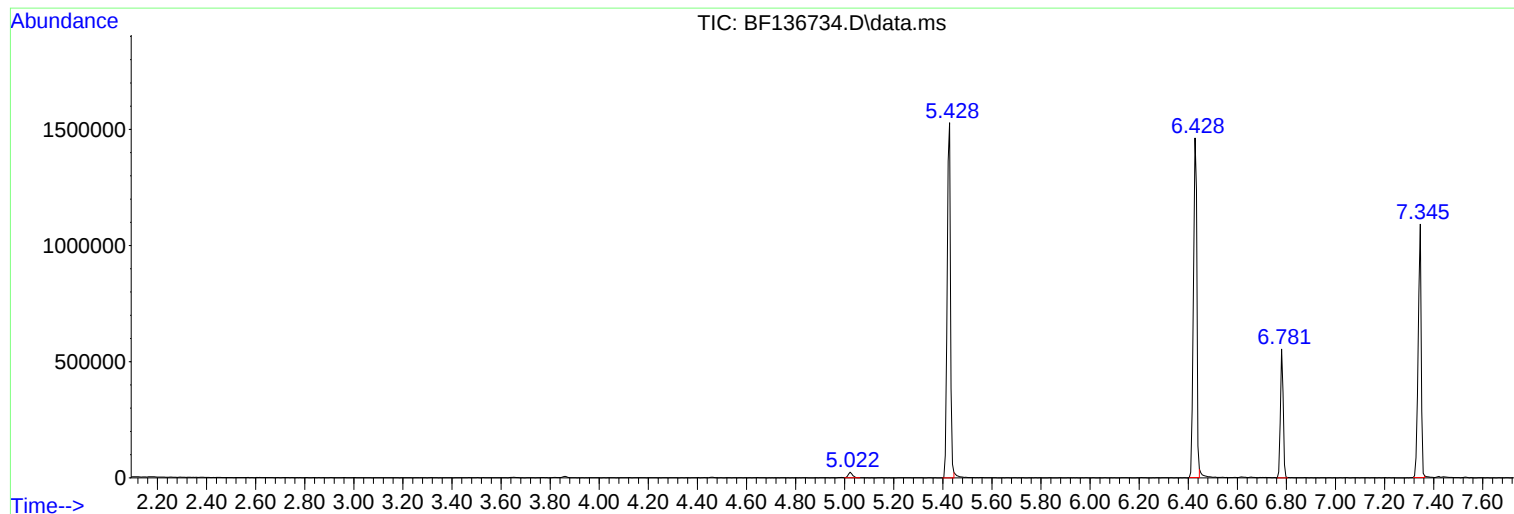
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ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HR-03-112223

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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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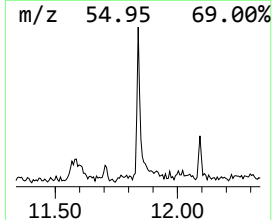
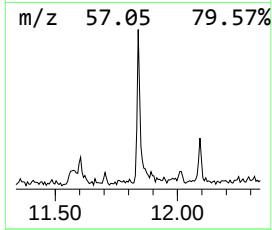
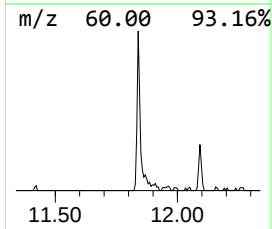
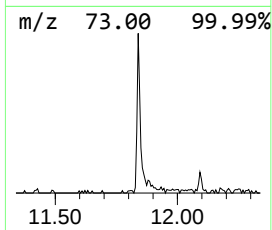
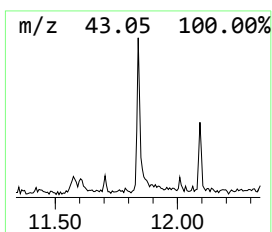
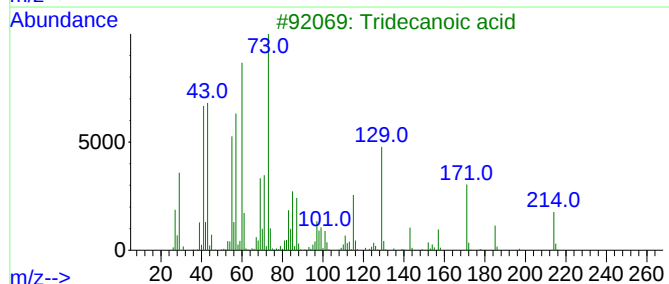
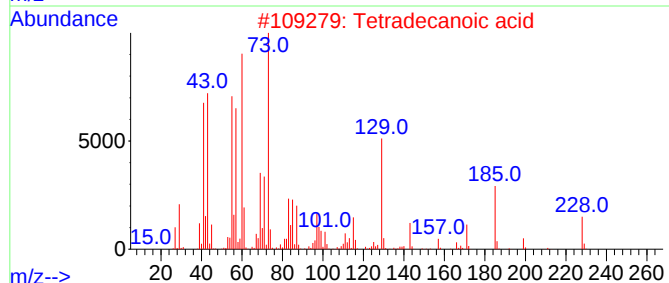
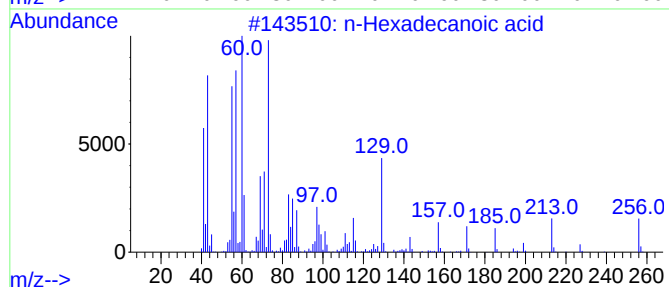
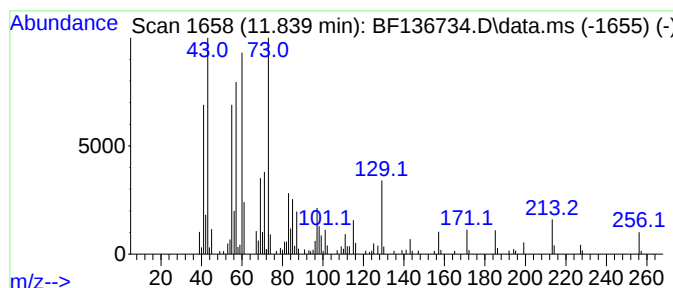
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.839	5.23 ng	118173	Phenanthrene-d10	11.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	97
3			Tridecanoic acid	214	C13H26O2	000638-53-9	96
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5			Undecanoic acid	186	C11H22O2	000112-37-8	64



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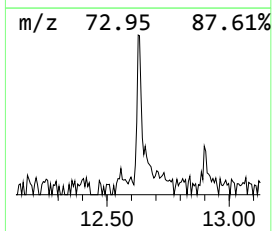
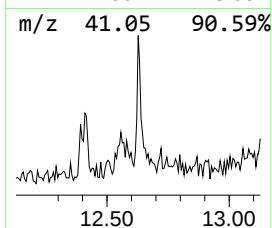
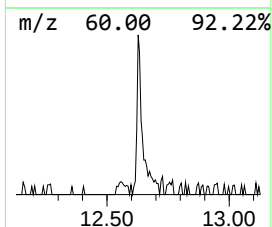
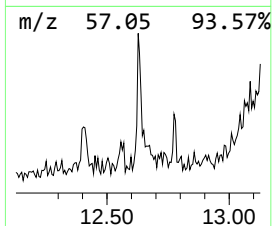
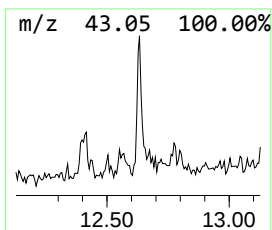
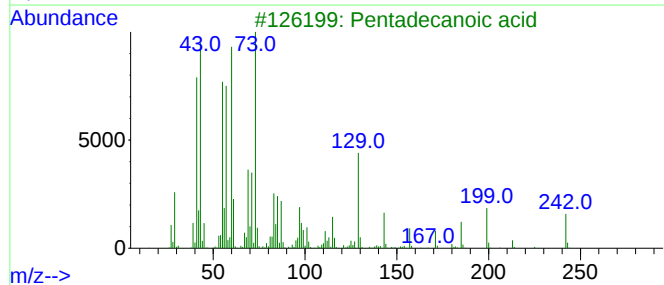
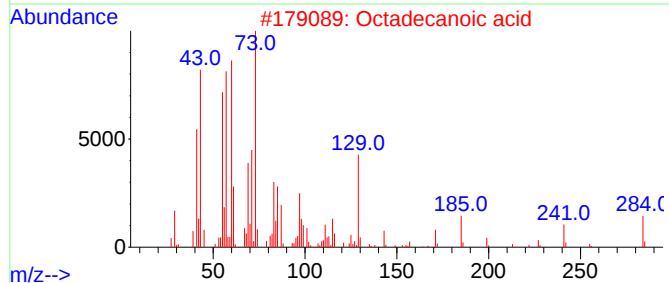
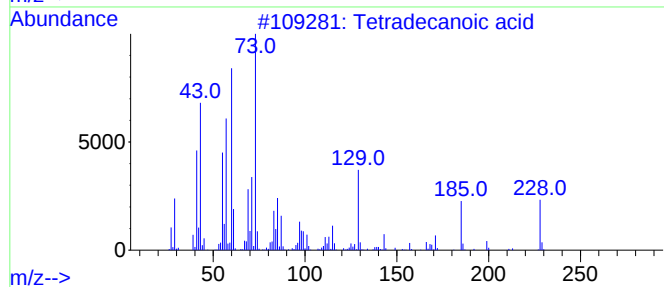
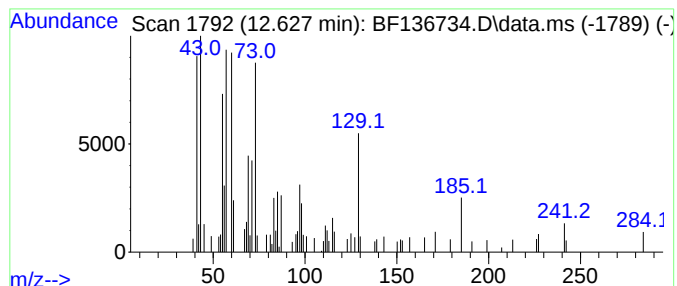
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Tetradecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.627	2.51 ng	56603	Phenanthrene-d10	11.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
2			Octadecanoic acid	284	C18H36O2	000057-11-4	60
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	53
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	50
5			n-Decanoic acid	172	C10H20O2	000334-48-5	50



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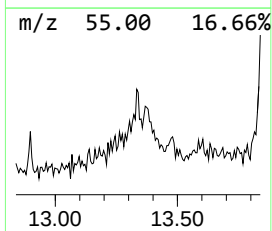
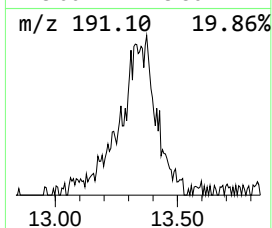
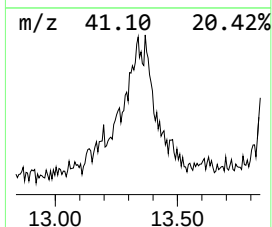
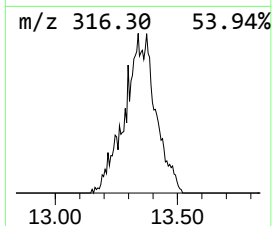
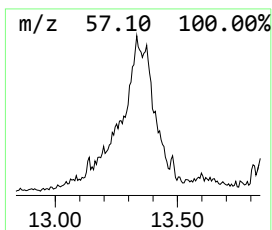
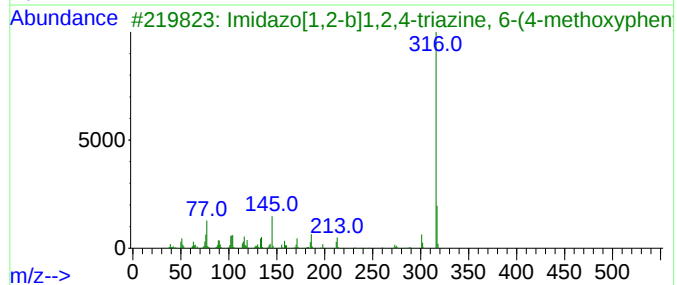
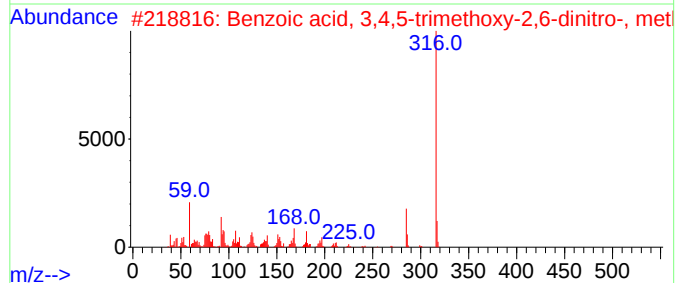
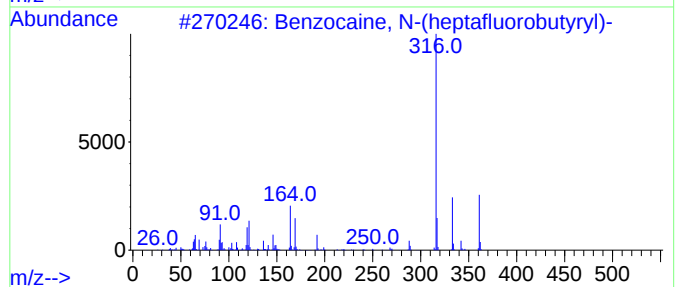
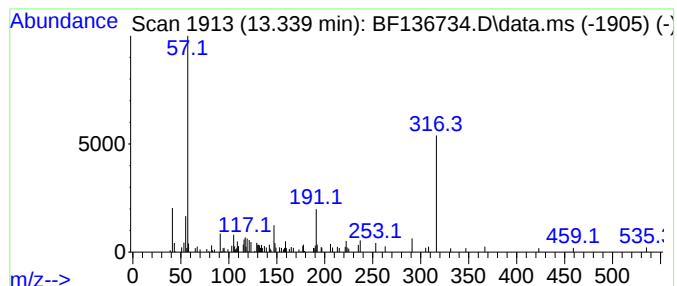
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 unknown13.339 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.339	2.07 ng	108721	Chrysene-d12	13.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzocaine, N-(heptafluorobutyryl)-	361	C13H10F7NO3	1000453-21-6	17
2			Benzoic acid, 3,4,5-trimethoxy-2...	316	C11H12N2O9	309922-16-5	16
3			Imidazo[1,2-b]1,2,4-triazine, 6-...	316	C19H16N4O	094103-49-8	16
4			2-Propyn-1-one, 1-(2-thienyl)-, ...	316	C13H8N4O4S	056588-20-6	12
5			D-Homoandrosta-4,17-dien-3-one, ...	316	C20H28O3	030298-69-2	12



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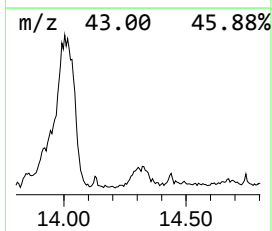
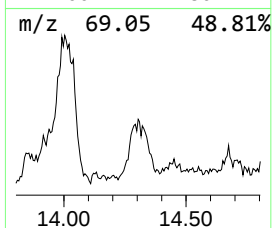
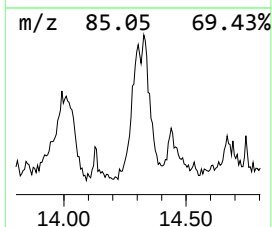
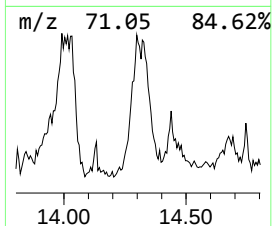
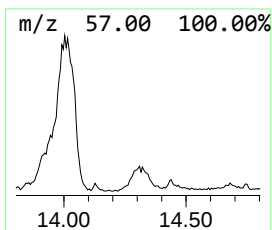
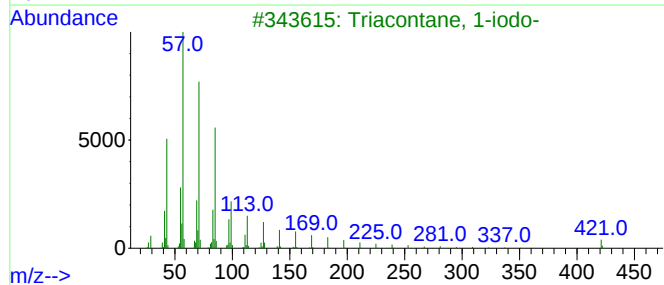
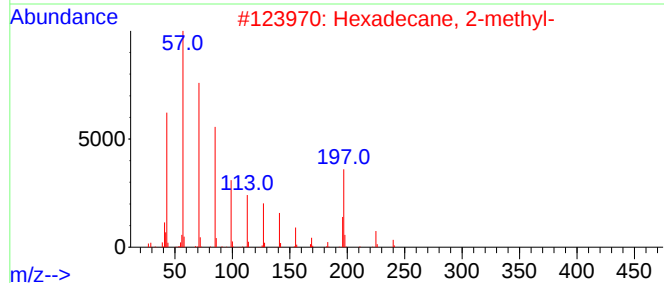
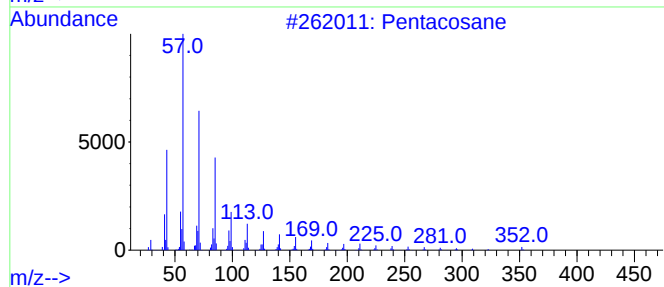
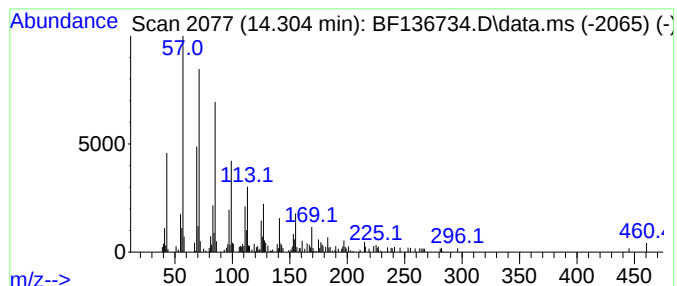
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Pentacosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.304	4.58 ng	240045	Chrysene-d12	13.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentacosane	352	C25H52	000629-99-2	87
2			Hexadecane, 2-methyl-	240	C17H36	001560-92-5	72
3			Triacontane, 1-iodo-	548	C30H61I	1000406-32-3	62
4			Octacosane, 1-iodo-	520	C28H57I	1000406-32-2	58
5			Pentadecane, 6-methyl-	226	C16H34	010105-38-1	58



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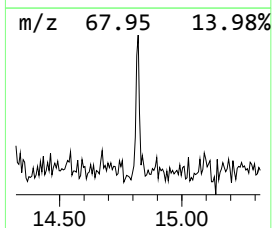
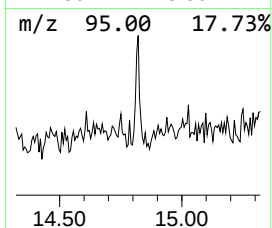
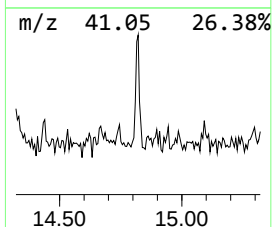
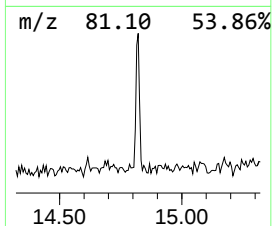
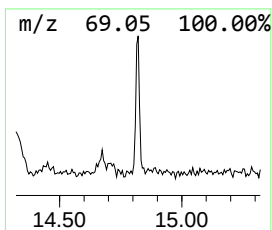
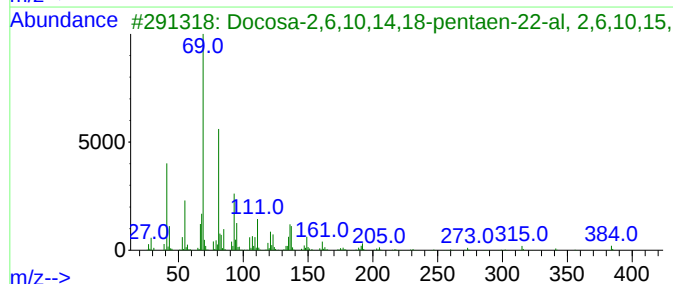
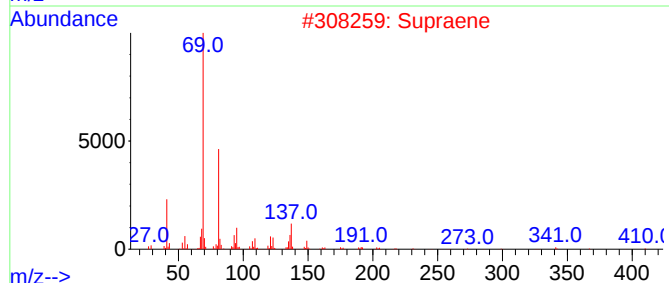
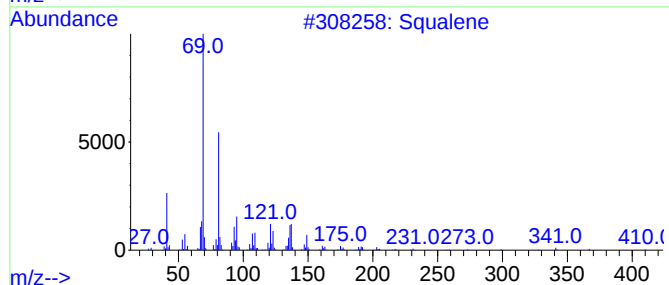
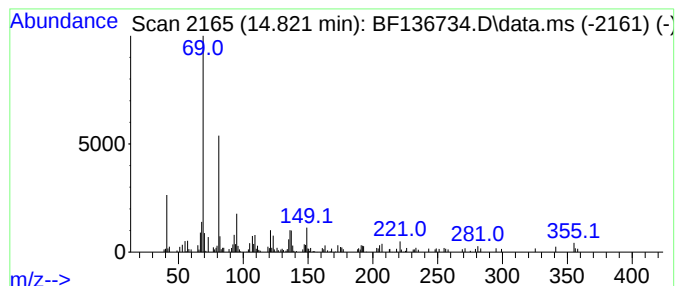
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.821	3.32 ng	64572	Perylene-d12	15.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Squalene	410	C30H50	000111-02-4	87
2			Supraene	410	C30H50	007683-64-9	83
3			Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	80
4			1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	72
5			Farnesol isomer a	222	C15H26O	1000108-92-4	64



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Hexadecanoic ...	11.839	5.2	ng	118173	4	11.304	451569	20.0
Tetradecanoic acid	12.627	2.5	ng	56603	4	11.304	451569	20.0
unknown13.339	13.339	2.1	ng	108721	5	13.963	1049320	20.0
Pentacosane	14.304	4.6	ng	240045	5	13.963	1049320	20.0
Squalene	14.821	3.3	ng	64572	6	15.439	388900	20.0