

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052623\
 Data File : BF133509.D
 Acq On : 26 May 2023 20:34
 Operator : CG\JU
 Sample : 02908-13
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TWP02

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-BF052523.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133509.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.211	17	21	34	rVB	47405	75081	1.95%	0.347%
2	3.899	303	308	313	rVB	42007	54998	1.43%	0.254%
3	4.416	392	396	402	rVB	58912	65989	1.72%	0.305%
4	5.040	497	502	506	rBV	871311	960971	25.00%	4.442%
5	5.440	566	570	574	rBV	1370860	1187105	30.89%	5.487%
6	6.452	738	742	745	rBV	860800	755100	19.65%	3.490%
7	6.834	804	807	811	rBV	1009686	801222	20.85%	3.704%
8	7.399	898	903	906	rBV	2237325	2326098	60.52%	10.753%
9	8.116	1022	1025	1029	rBV	1180627	1044799	27.19%	4.830%
10	9.198	1204	1209	1212	rBV	4464874	3843220	100.00%	17.765%
11	9.875	1320	1324	1327	rBV	1346490	1100364	28.63%	5.086%
12	10.587	1442	1445	1449	rBV	630371	530166	13.79%	2.451%
13	10.663	1453	1458	1461	rBV	1799201	1723083	44.83%	7.965%
14	10.898	1492	1498	1502	rBV	83256	72888	1.90%	0.337%
15	11.357	1573	1576	1580	rVB	1256388	1141578	29.70%	5.277%
16	11.886	1663	1666	1671	rBV	161638	172508	4.49%	0.797%
17	12.675	1797	1800	1807	rBV2	42261	51879	1.35%	0.240%
18	12.951	1843	1847	1851	rBV	3530997	3690623	96.03%	17.060%
19	13.863	1998	2002	2012	rBV2	132480	203795	5.30%	0.942%
20	14.004	2022	2026	2029	rBV	1015365	942789	24.53%	4.358%
21	14.869	2169	2173	2177	rVB	78817	82068	2.14%	0.379%
22	15.463	2268	2274	2279	rBV	621940	760027	19.78%	3.513%
23	15.510	2279	2282	2289	rVB	36039	46711	1.22%	0.216%

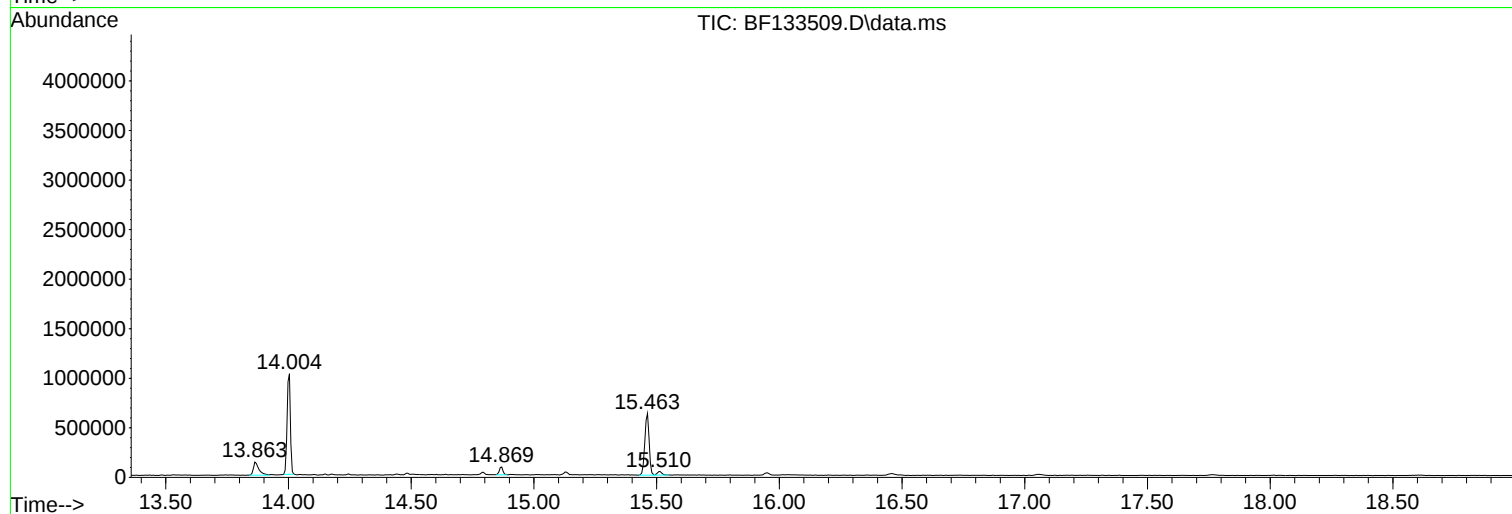
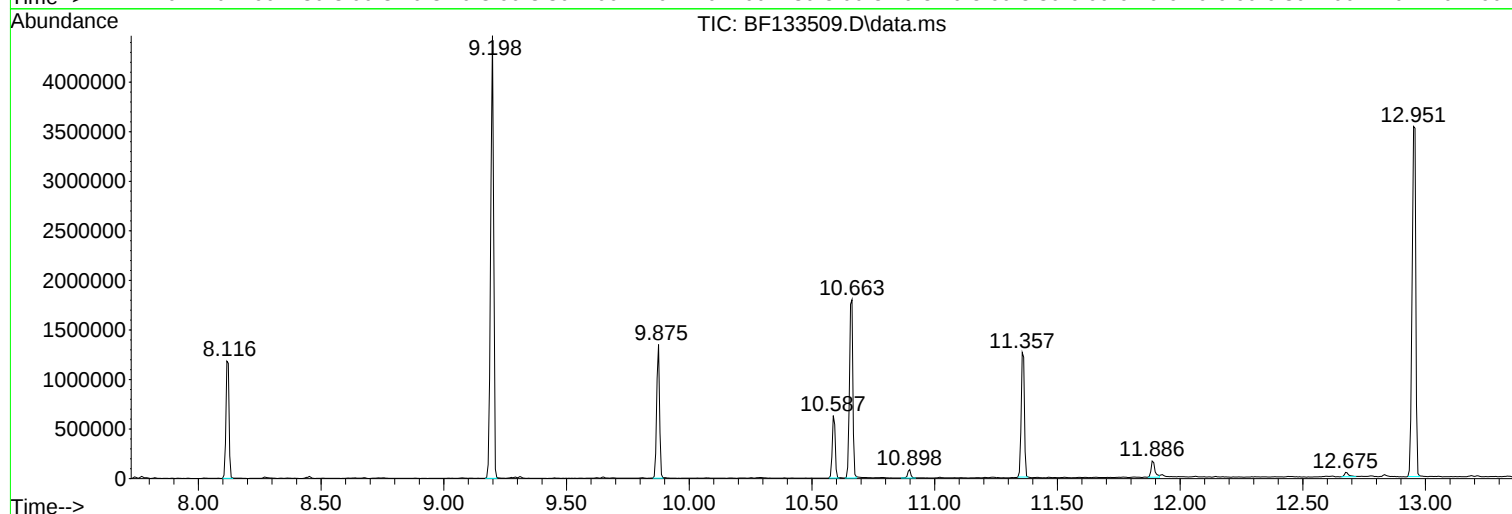
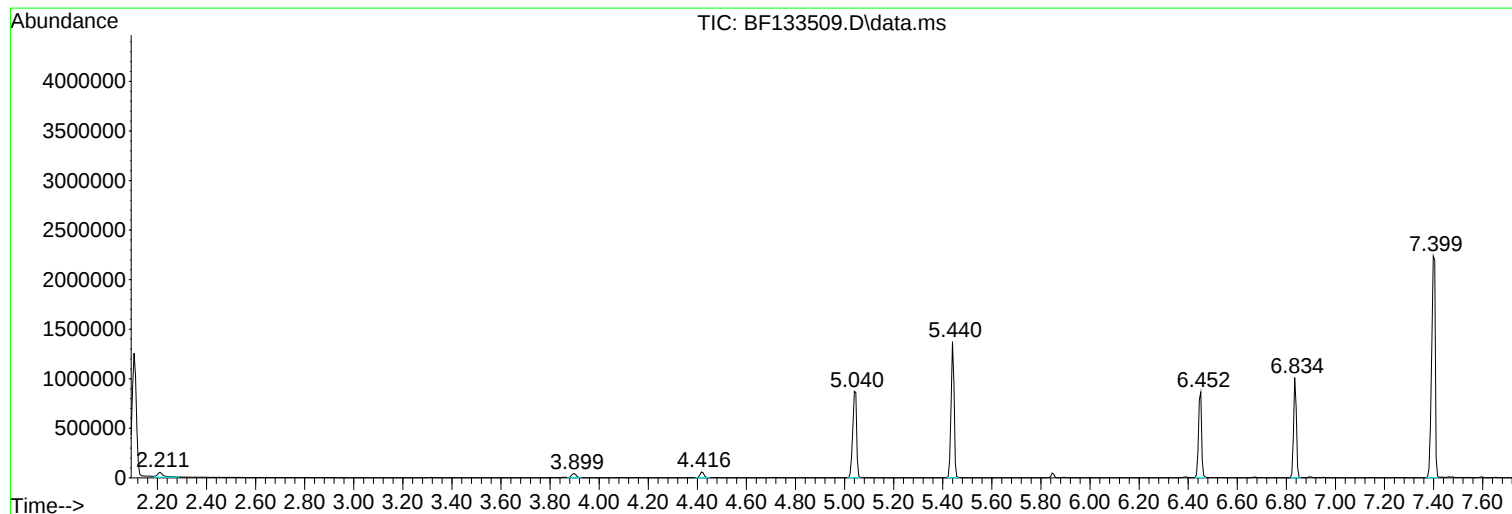
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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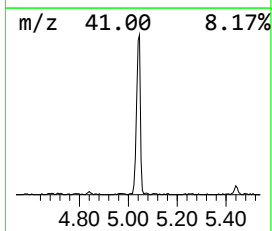
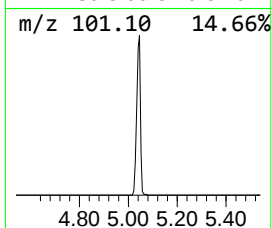
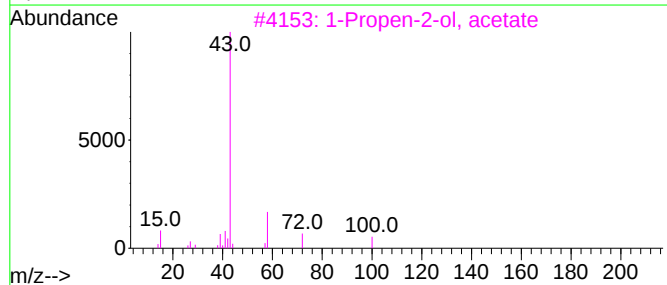
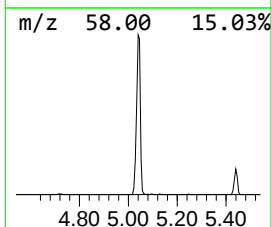
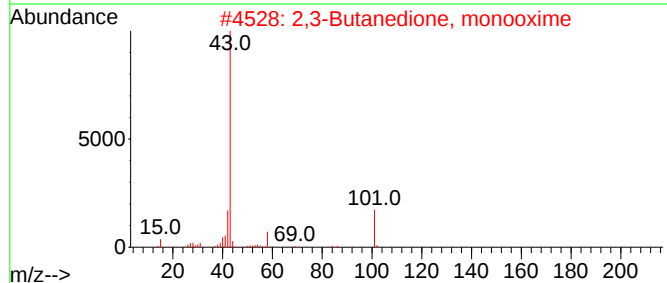
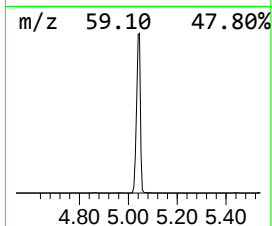
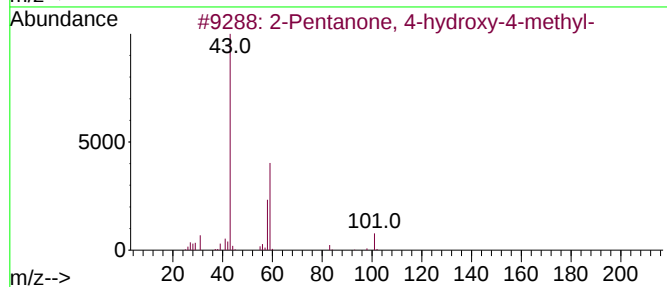
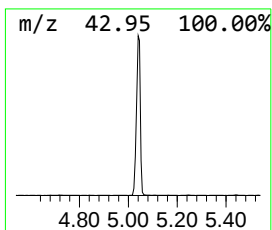
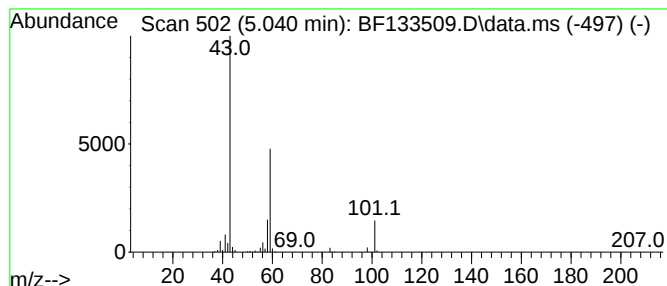
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052523.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.040	23.99 ng	960971	1,4-Dichlorobenzene-d4	6.834

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64		
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27		
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12		
4	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9		
5	Allyl acetate	100	C5H8O2	000591-87-7	9		



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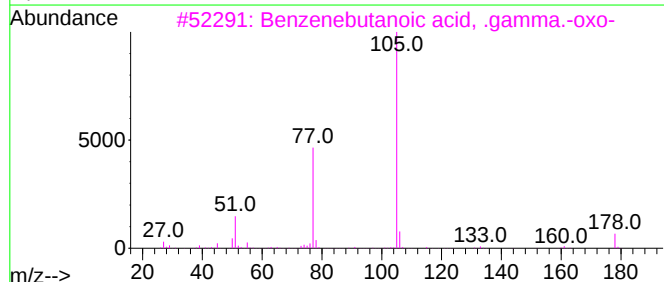
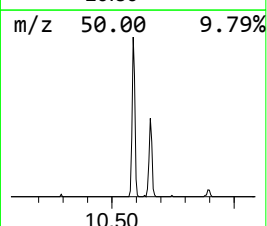
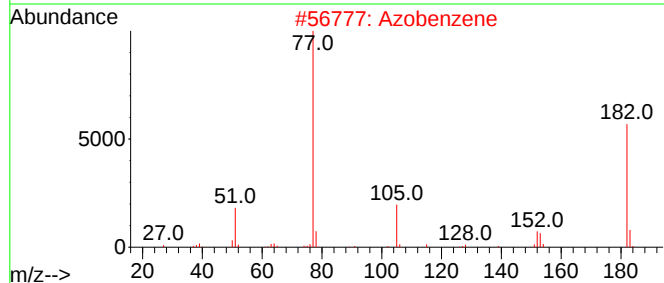
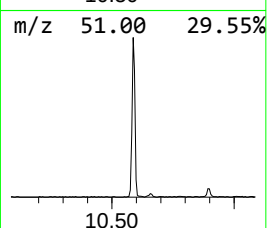
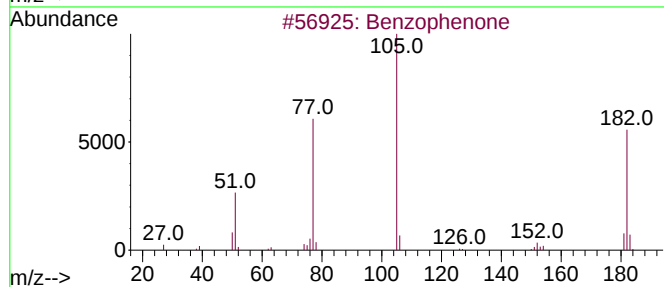
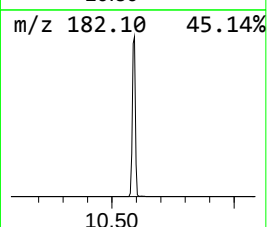
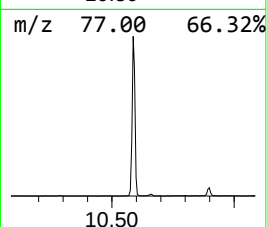
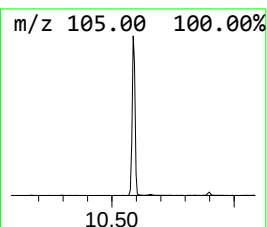
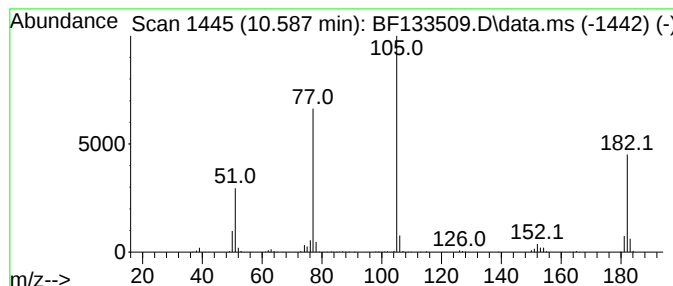
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Peak Number 2 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.587	9.64 ng	530166	Acenaphthene-d10	9.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Azobenzene	182	C12H10N2	000103-33-3	53
3			Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	50
4			Benzenoacetic acid, .alpha.-oxo-...	178	C10H10O3	001603-79-8	50
5			Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	50



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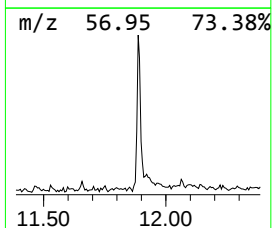
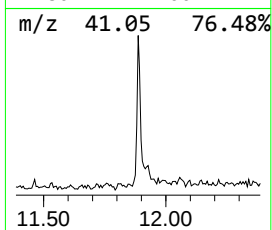
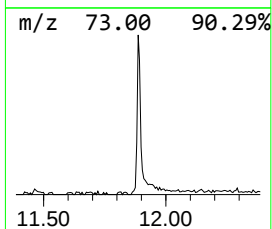
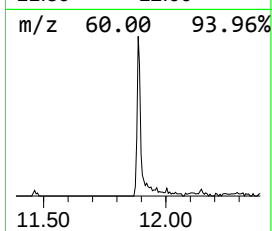
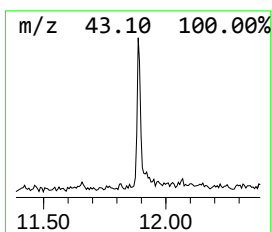
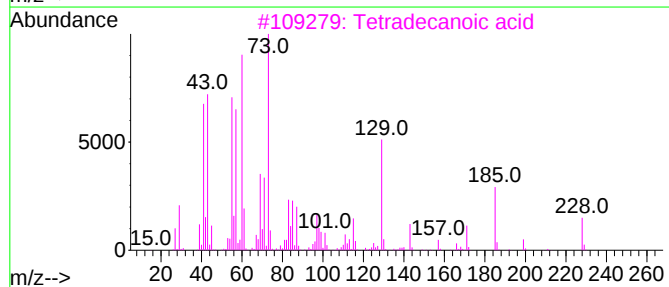
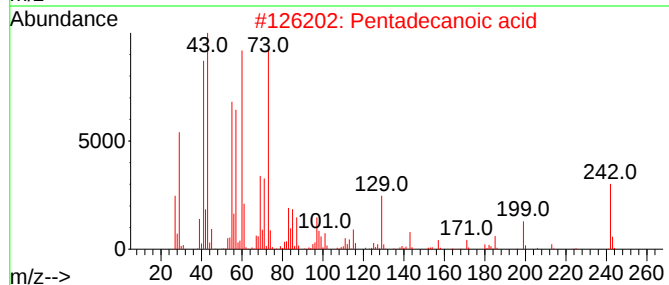
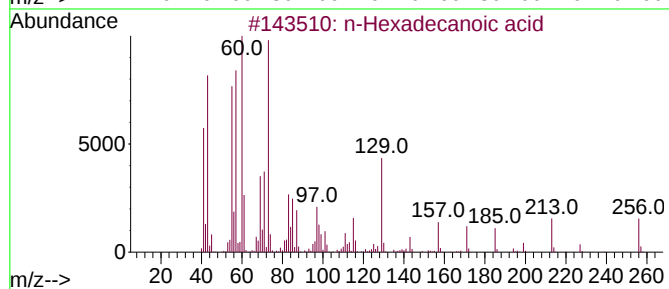
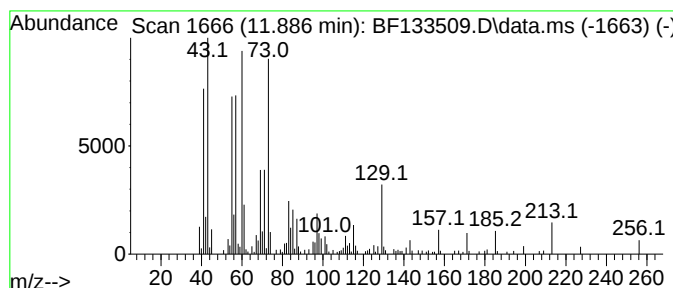
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.887	3.02 ng	172508	Phenanthrene-d10	11.363

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4		n-Decanoic acid	172	C10H20O2	000334-48-5	86
5		Tridecanoic acid	214	C13H26O2	000638-53-9	64



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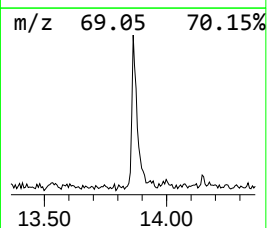
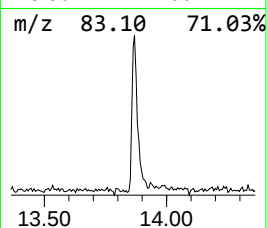
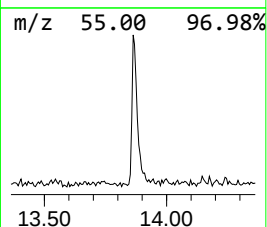
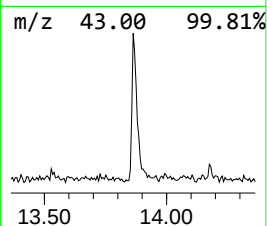
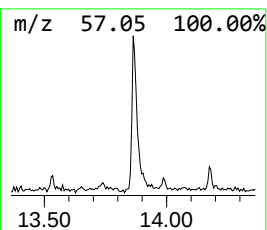
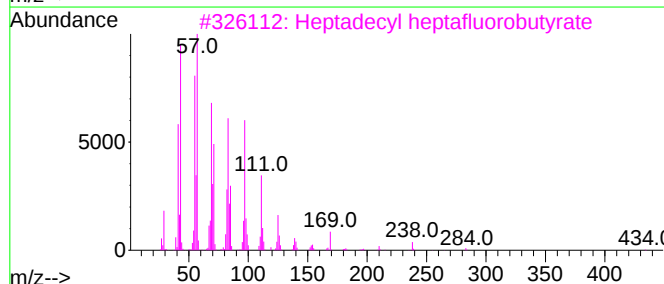
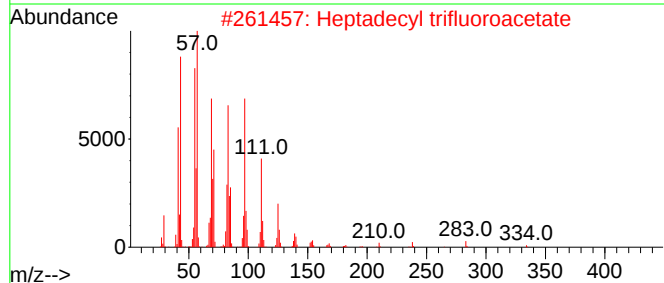
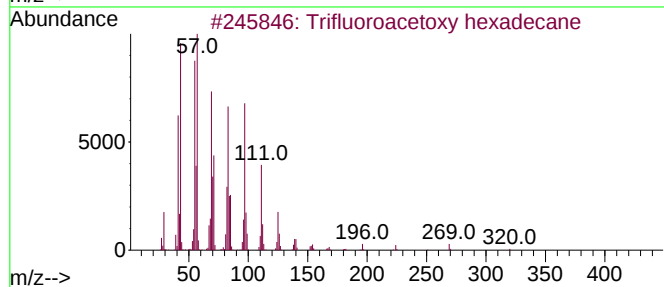
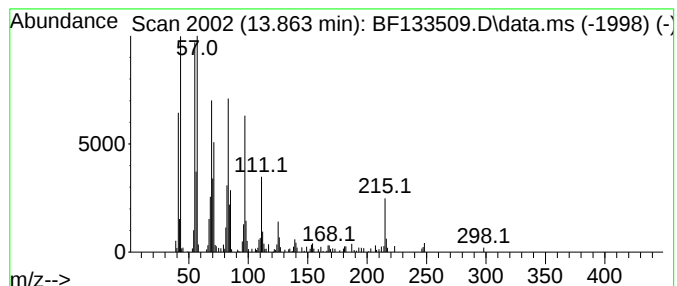
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Peak Number 4 Trifluoroacetoxy hexadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.863	4.32 ng	203795	Chrysene-d12	14.004

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
2			Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	91
3			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
4			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
5			Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	91



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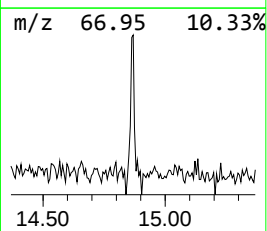
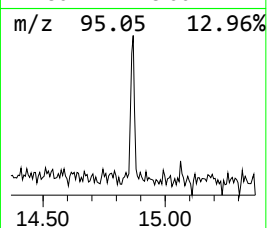
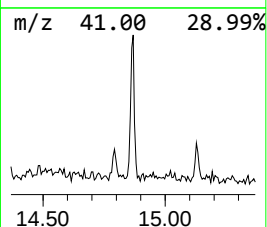
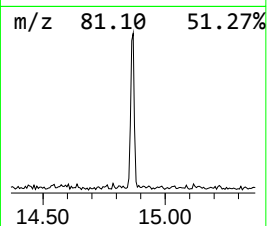
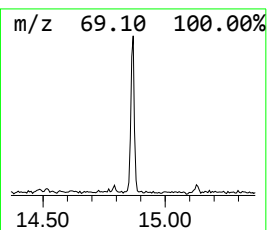
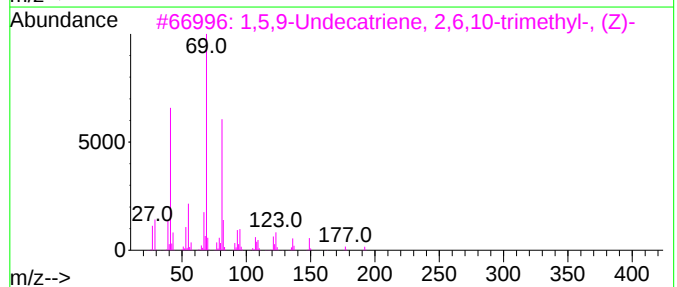
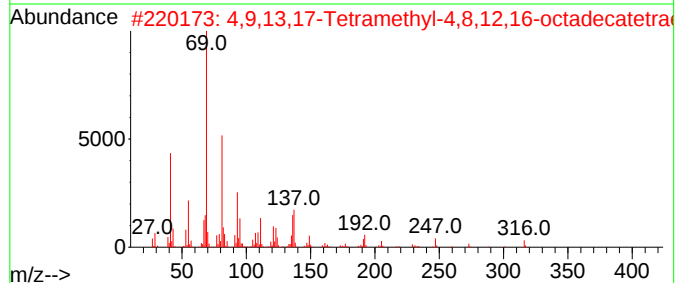
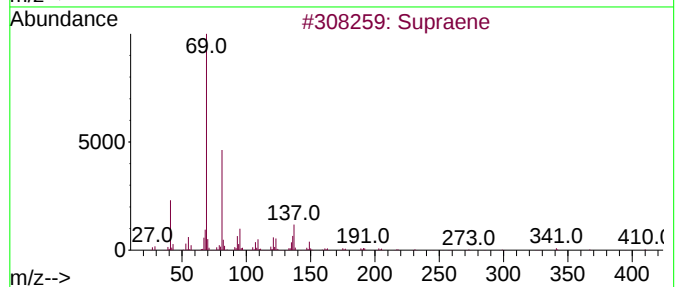
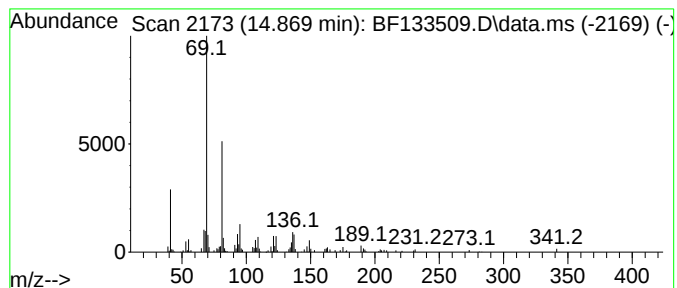
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Peak Number 5 Supraene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.869	2.16 ng	82068	Perylene-d12	15.463

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	90
2			4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	83
3			1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	80
4			6,10,14-Hexadecatrien-1-ol, 3,7,...	292	C20H36O	036237-66-8	78
5			Hexadeca-2,6,10,14-tetraen-1-ol,...	290	C20H34O	007614-21-3	72



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.040	24.0	ng	960971	1	6.834	801222	20.0
Benzophenone	10.587	9.6	ng	530166	3	9.875	1100360	20.0
n-Hexadecanoic ...	11.887	3.0	ng	172508	4	11.363	1141580	20.0
Trifluoroacetox...	13.863	4.3	ng	203795	5	14.004	942789	20.0
Supraene	14.869	2.2	ng	82068	6	15.463	760027	20.0