

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF053023\
 Data File : BF133525.D
 Acq On : 30 May 2023 16:48
 Operator : CG\JU
 Sample : 02957-04
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-10-0A

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: BF133525.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.051	498	504	512	rVB	90443	113854	3.45%	0.470%
2	5.445	565	571	574	rBV	3027361	2945350	89.13%	12.153%
3	6.457	737	743	746	rBV	2927127	3081530	93.25%	12.715%
4	6.833	803	807	810	rBV	1014025	909782	27.53%	3.754%
5	7.392	897	902	905	rBV	1955040	1783885	53.98%	7.360%
6	8.116	1021	1025	1028	rBV	1414301	1185547	35.88%	4.892%
7	9.192	1204	1208	1211	rVB	3655731	2962697	89.65%	12.224%
8	9.869	1319	1323	1326	rBV	1624748	1257158	38.04%	5.187%
9	10.586	1441	1445	1448	rBV	378574	293088	8.87%	1.209%
10	10.657	1453	1457	1460	rBV	2501225	2219418	67.16%	9.157%
11	11.357	1572	1576	1579	rBV	1640944	1347053	40.76%	5.558%
12	11.886	1662	1666	1670	rBV	255597	228688	6.92%	0.944%
13	12.674	1795	1800	1805	rBV3	40956	50130	1.52%	0.207%
14	12.951	1842	1847	1850	rBV	3304893	3304560	100.00%	13.635%
15	13.180	1881	1886	1889	rBV	35598	35754	1.08%	0.148%
16	13.851	1997	2000	2014	rBV	199359	331542	10.03%	1.368%
17	13.998	2021	2025	2028	rBV	1270526	1122154	33.96%	4.630%
18	14.174	2051	2055	2065	rVB	48898	53795	1.63%	0.222%
19	14.480	2103	2107	2119	rBV	45187	60526	1.83%	0.250%
20	14.762	2151	2155	2157	rBV	138870	139458	4.22%	0.575%
21	15.456	2268	2273	2278	rBV	659171	810248	24.52%	3.343%

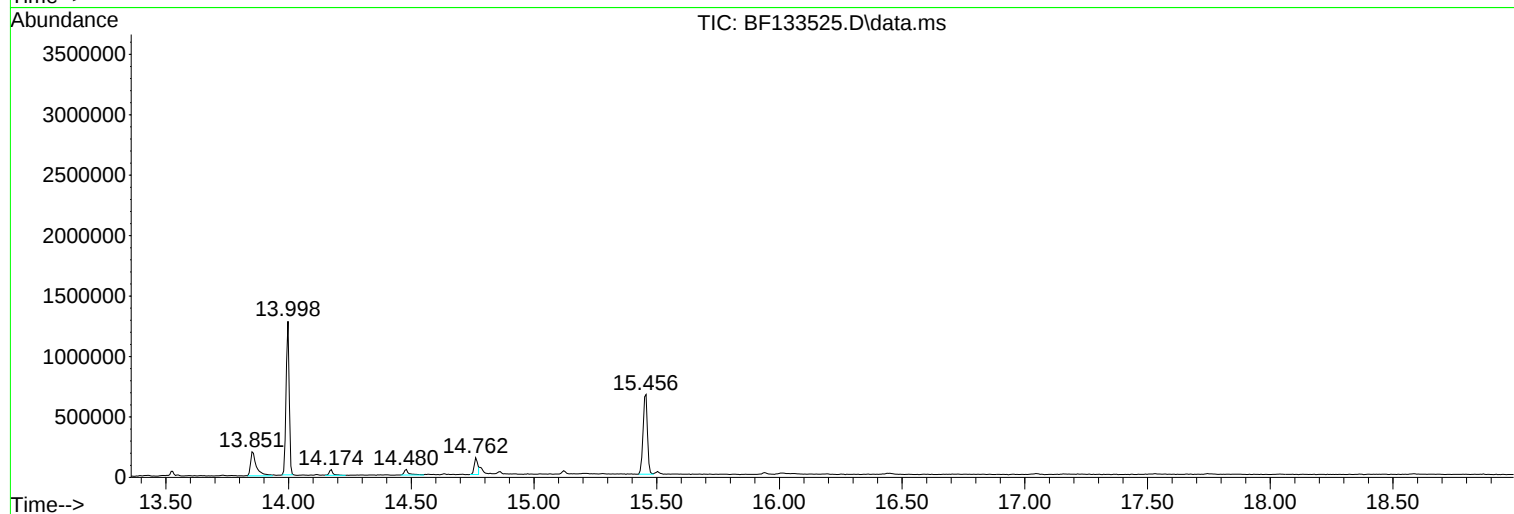
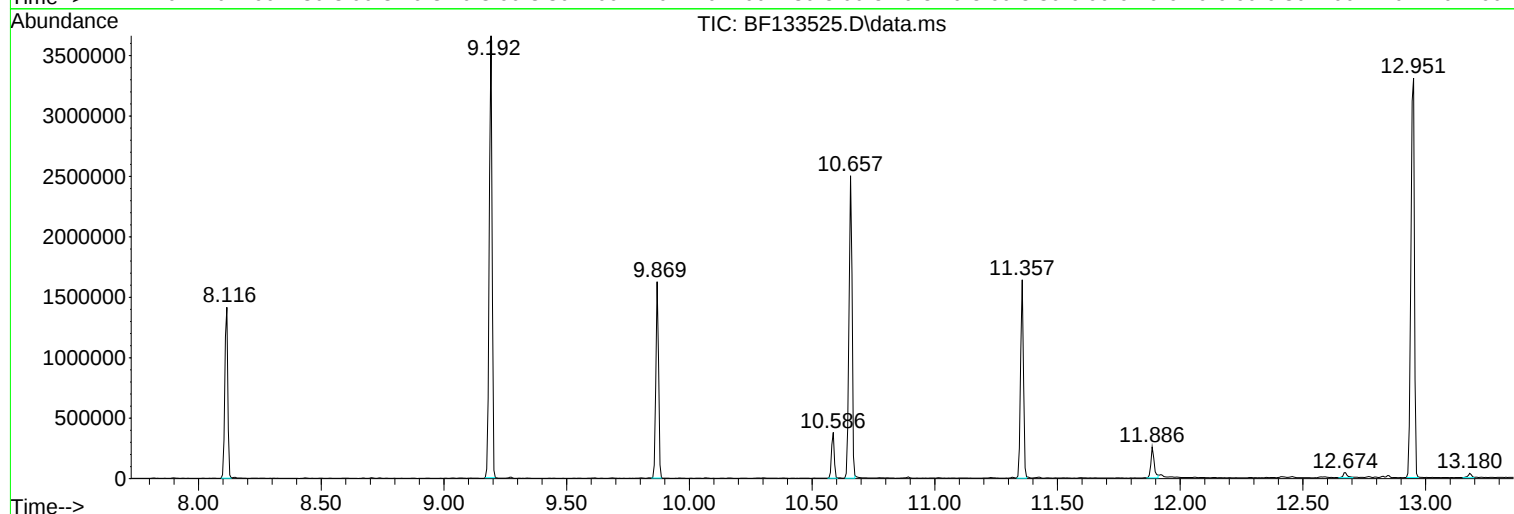
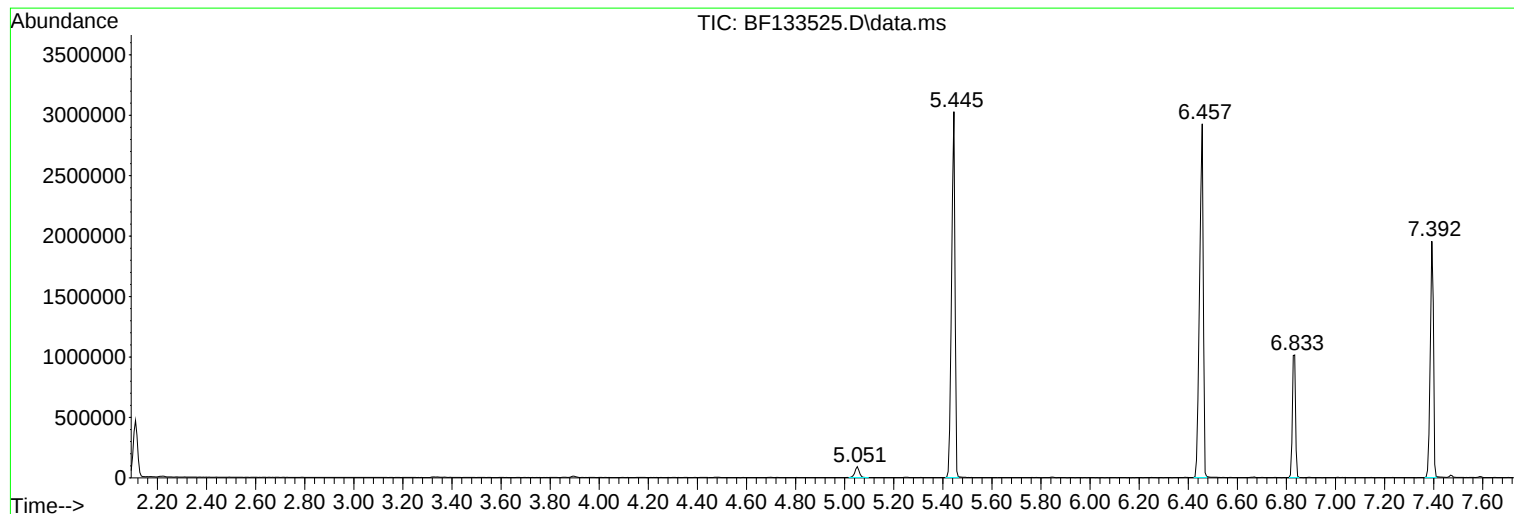
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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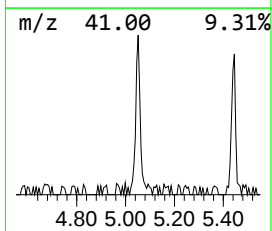
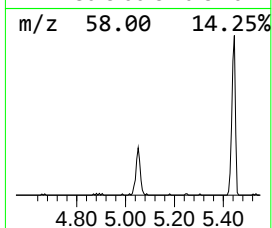
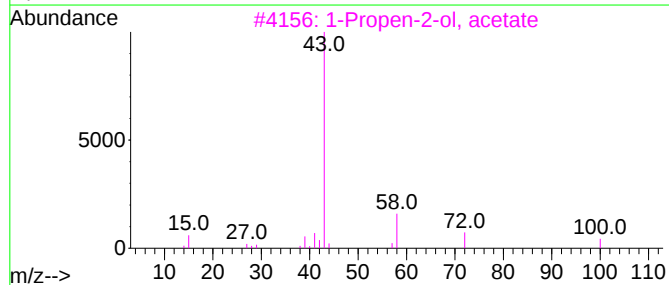
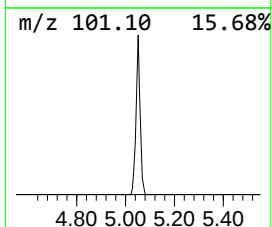
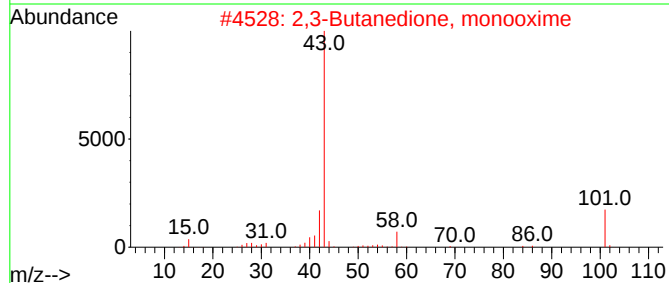
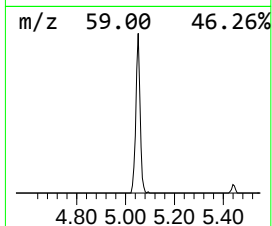
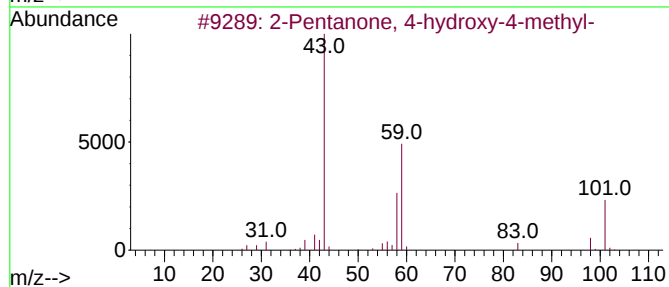
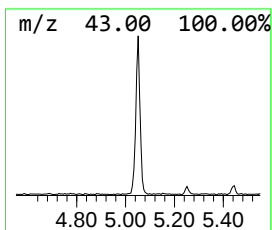
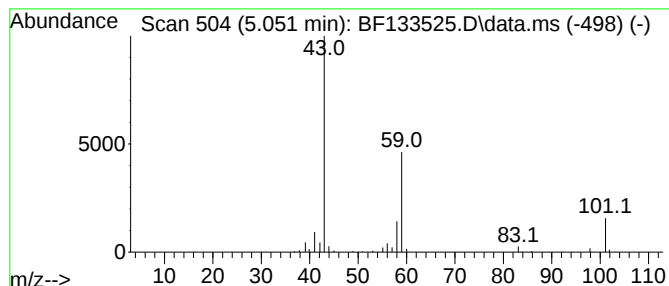
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.051	2.50 ng	113854	1,4-Dichlorobenzene-d4	6.833

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72		
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	30		
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12		
4	Acetamide, N-(aminocarbonyl)-	102	C3H6N2O2	000591-07-1	9		
5	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9		



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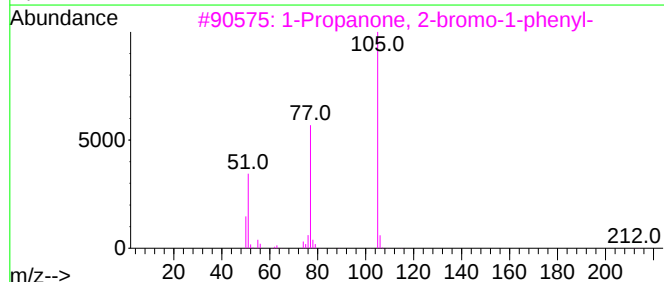
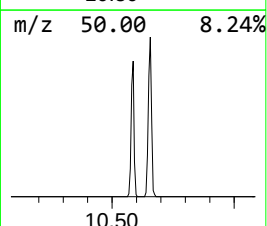
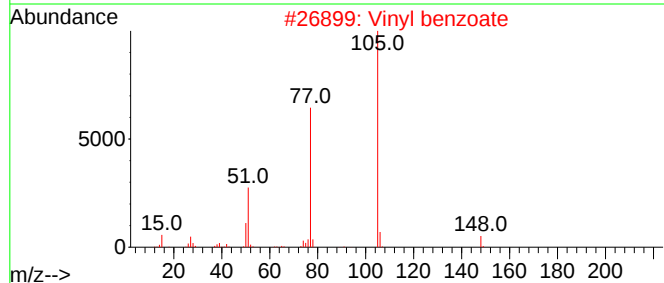
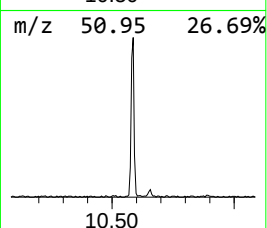
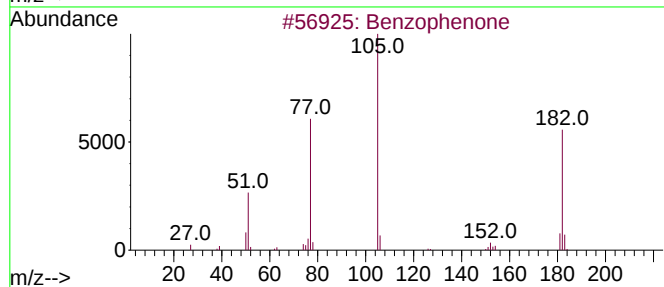
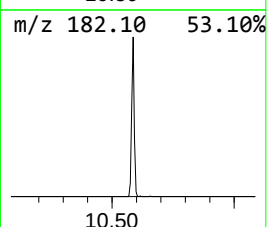
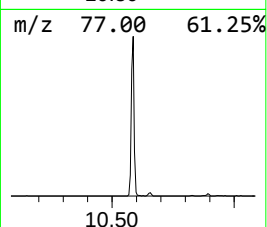
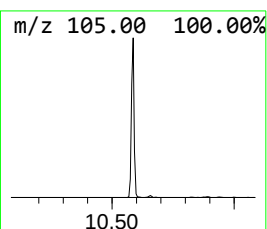
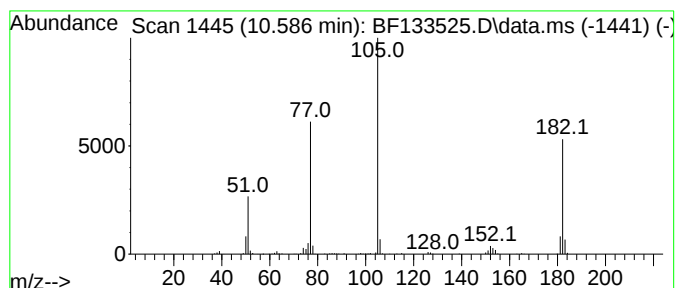
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.586	4.66 ng	293088	Acenaphthene-d10	9.869

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Vinyl benzoate	148	C9H8O2	000769-78-8	47
3			1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47
4			N-Methylbenzamide, N-chlorodiflu...	247	C10H8ClF2NO2	1000446-98-2	47
5			N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	47



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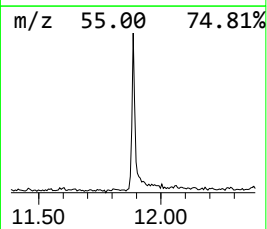
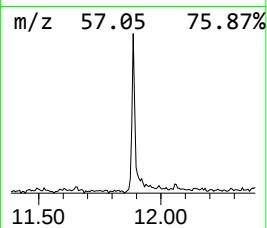
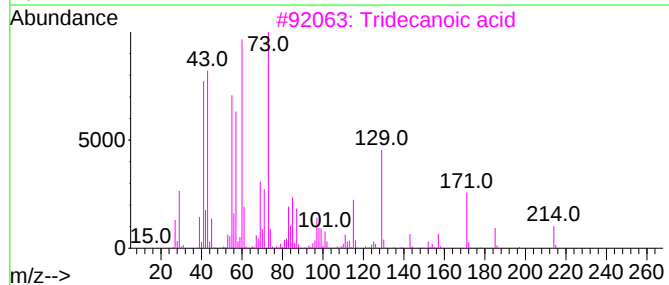
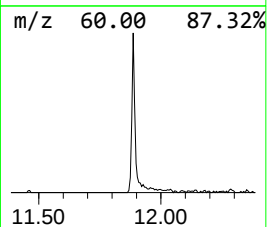
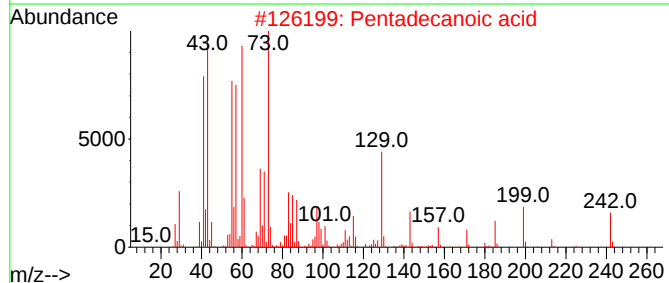
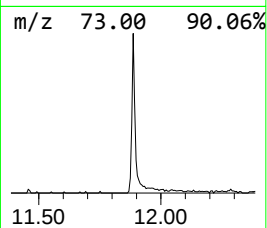
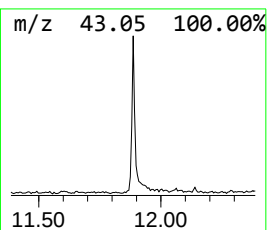
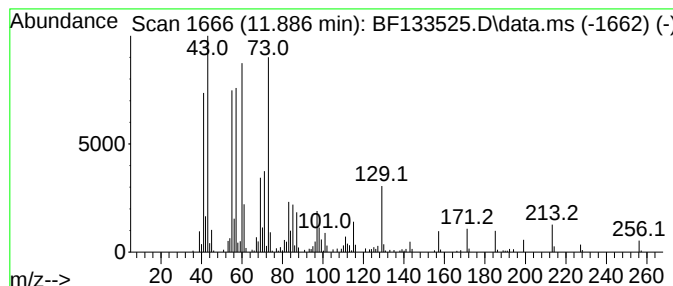
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.886	3.40 ng	228688	Phenanthrene-d10	11.357

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	90
3			Tridecanoic acid	214	C13H26O2	000638-53-9	90
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5			Isopropyl palmitate	298	C19H38O2	000142-91-6	64



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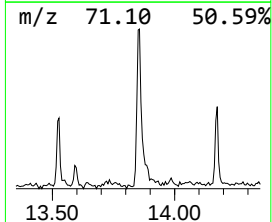
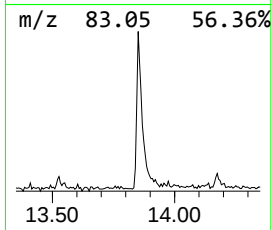
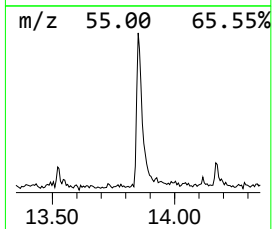
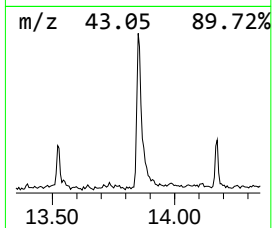
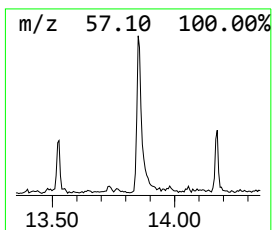
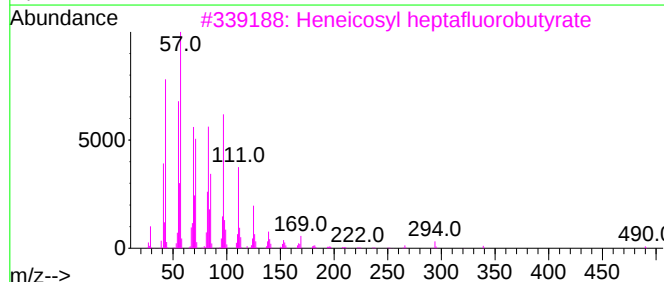
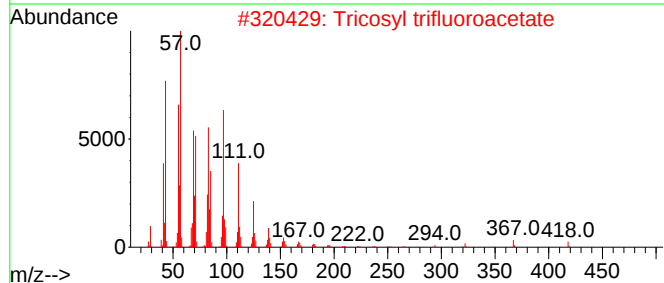
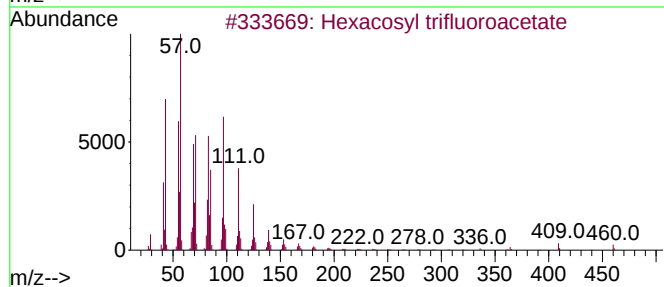
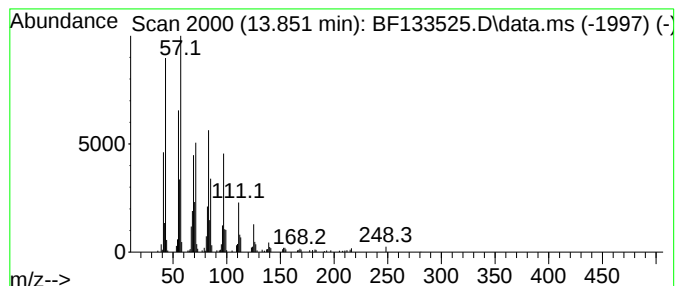
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Peak Number 4 Hexacosyl trifluoroacetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.851	5.91 ng	331542	Chrysene-d12	13.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosyl trifluoroacetate	478	C28H53F3O2	1000351-75-0	91
2			Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	91
3			Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	91
4			Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	91
5			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91



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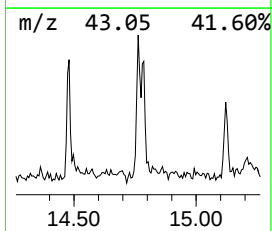
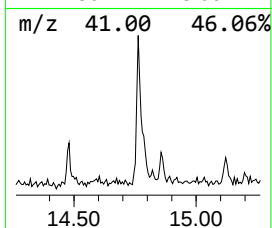
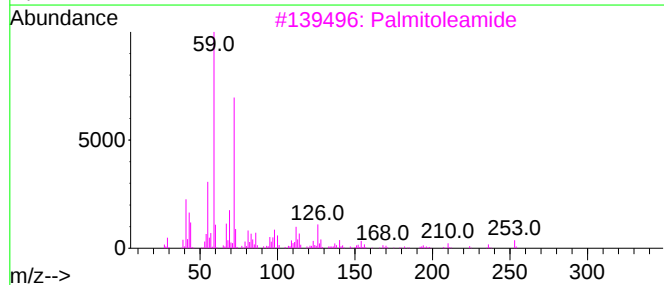
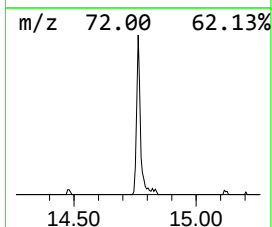
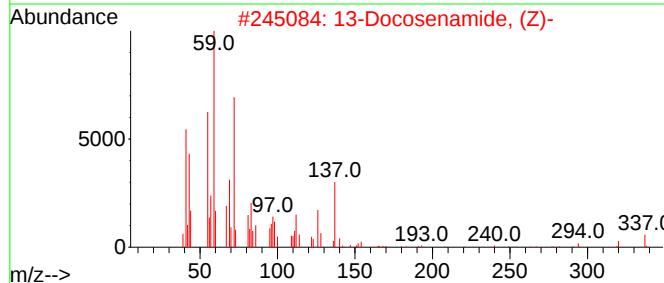
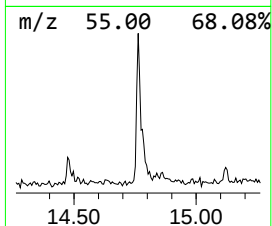
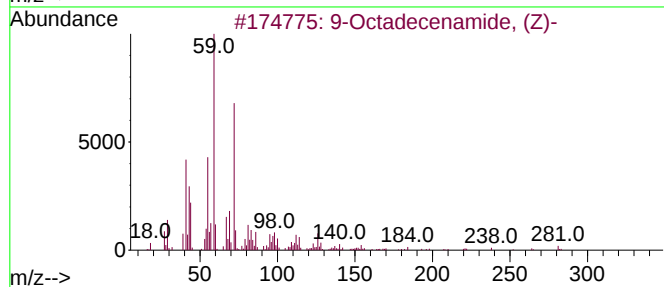
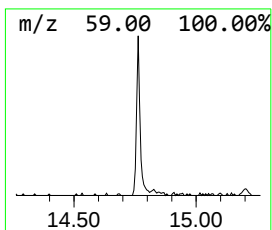
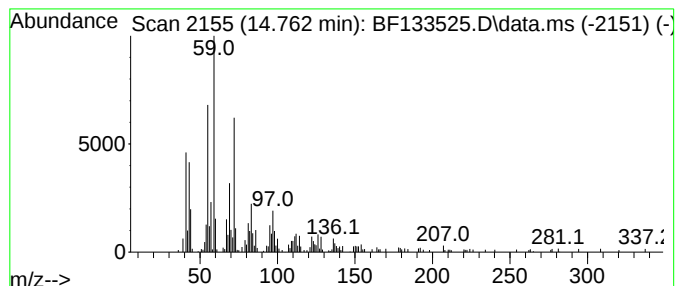
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Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.762	3.44 ng	139458	Perylene-d12	15.456

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	96
2			13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	80
3			Palmitoleamide	253	C16H31NO	106010-22-4	58
4			7-Nonenamide	155	C9H17NO	090949-53-4	53
5			9-Octadecenamide	281	C18H35NO	003322-62-1	46



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.051	2.5	ng	113854	1	6.833	909782	20.0
Benzophenone	10.586	4.7	ng	293088	3	9.869	1257160	20.0
n-Hexadecanoic ...	11.886	3.4	ng	228688	4	11.357	1347050	20.0
Hexacosyl trifl...	13.851	5.9	ng	331542	5	13.998	1122150	20.0
9-Octadecenamid...	14.762	3.4	ng	139458	6	15.456	810248	20.0