

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102924\
 Data File : BF140131.D
 Acq On : 29 Oct 2024 23:49
 Operator : RC/JU
 Sample : P4594-13
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-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_F\Methods\8270-BF101824.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF140131.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.187	9	16	29	rVB	926900	1458672	71.99%	8.987%
2	5.110	506	513	520	rVB3	11312	22170	1.09%	0.137%
3	5.504	574	580	585	rBV	1418602	1845518	91.08%	11.370%
4	6.504	744	750	774	rVB	1414840	1967439	97.10%	12.121%
5	6.886	810	815	821	rBV	631619	780761	38.53%	4.810%
6	7.445	904	910	915	rBV	932209	1183656	58.42%	7.292%
7	7.698	948	953	965	rVB	52264	65367	3.23%	0.403%
8	8.169	1027	1033	1038	rBV	811175	1009180	49.80%	6.217%
9	8.380	1065	1069	1079	rVB	17134	23348	1.15%	0.144%
10	9.239	1210	1215	1226	rBV	1536952	2026270	100.00%	12.484%
11	9.922	1326	1331	1343	rBV	803050	1021682	50.42%	6.294%
12	10.633	1447	1452	1460	rBV	117922	146155	7.21%	0.900%
13	10.710	1460	1465	1479	rVV	714093	921515	45.48%	5.677%
14	11.410	1579	1584	1592	rBV	652046	807238	39.84%	4.973%
15	11.933	1668	1673	1689	rBV2	53093	100848	4.98%	0.621%
16	12.992	1848	1853	1868	rBV	1048100	1384188	68.31%	8.528%
17	13.898	2001	2007	2022	rBV	34367	93786	4.63%	0.578%
18	14.051	2028	2033	2045	rVB	542330	705638	34.82%	4.347%
19	14.909	2175	2179	2184	rVB	18815	24651	1.22%	0.152%
20	15.539	2279	2286	2299	rBV	390742	643338	31.75%	3.964%

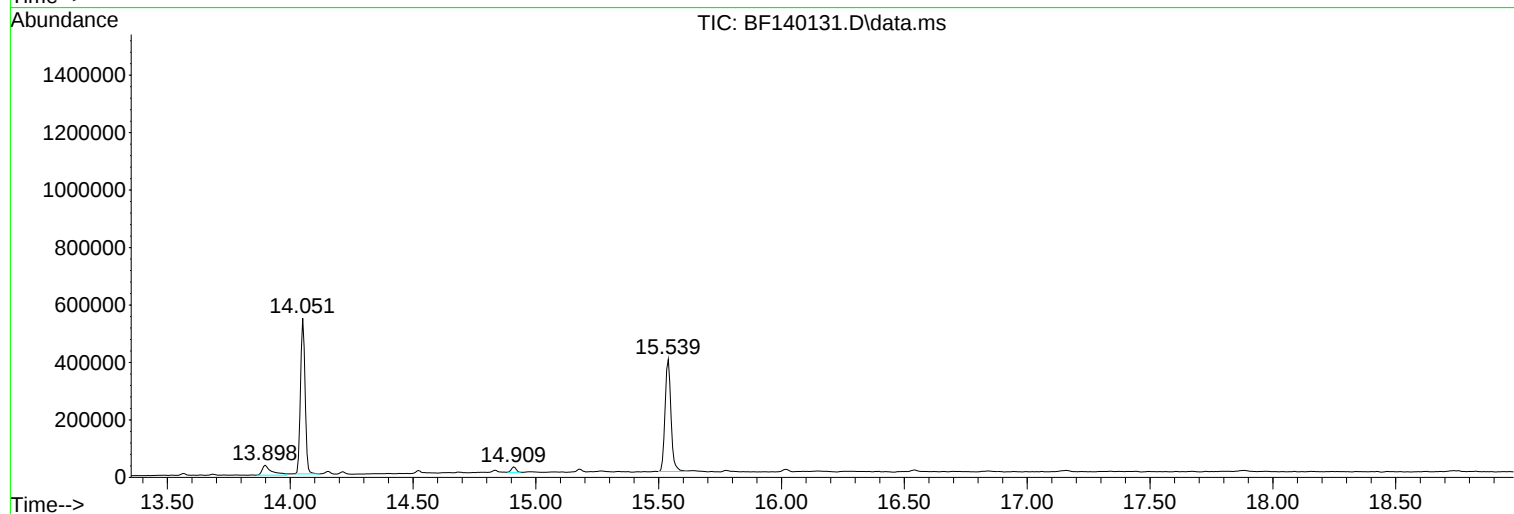
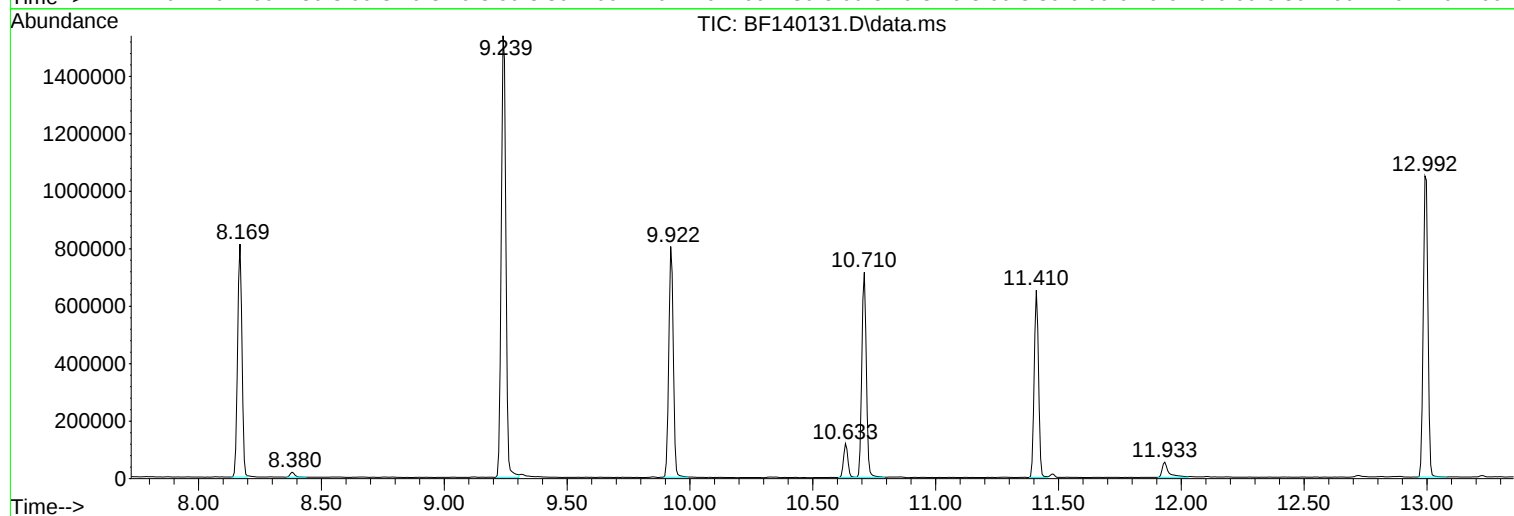
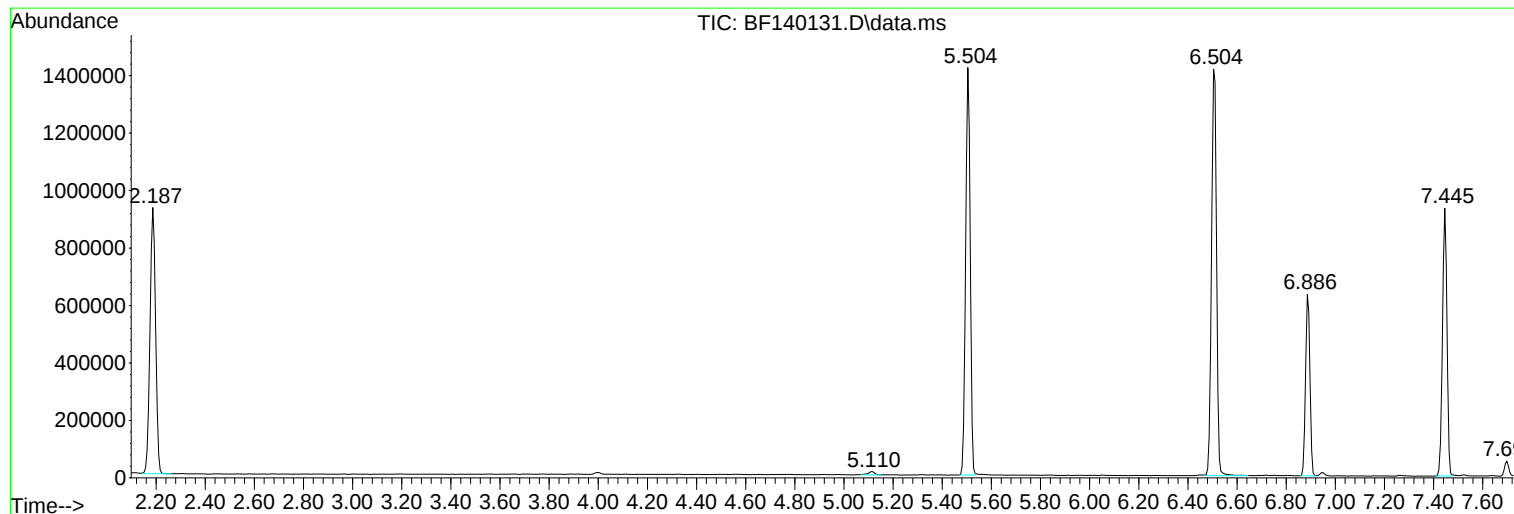
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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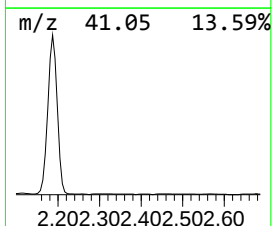
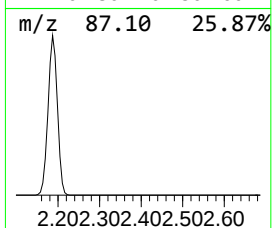
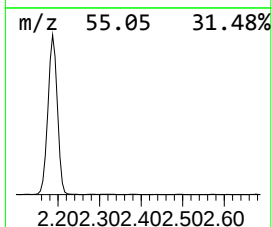
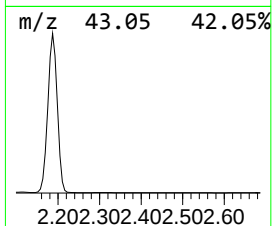
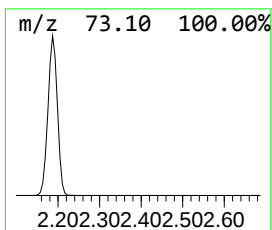
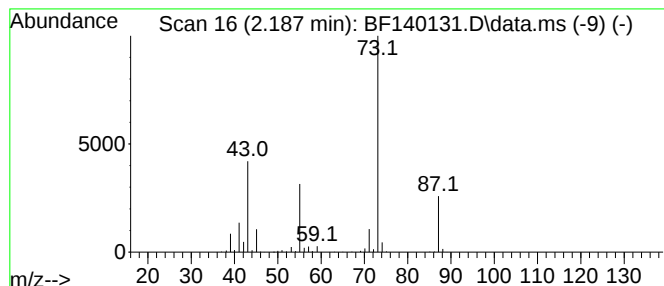
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.187	37.37 ng	1458670	1,4-Dichlorobenzene-d4	6.886

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4			Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	17
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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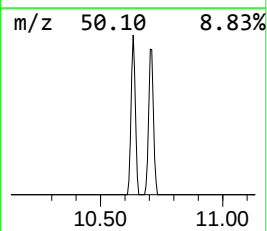
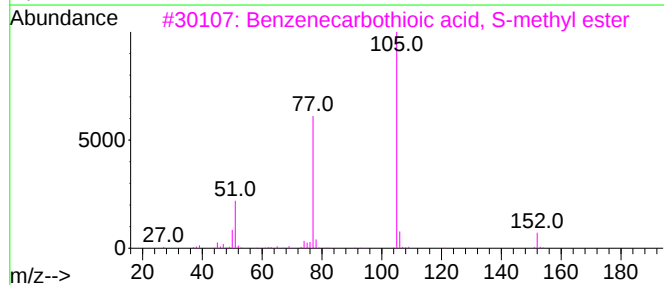
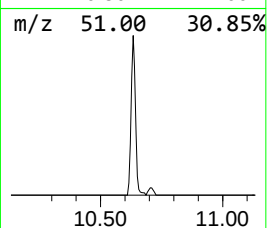
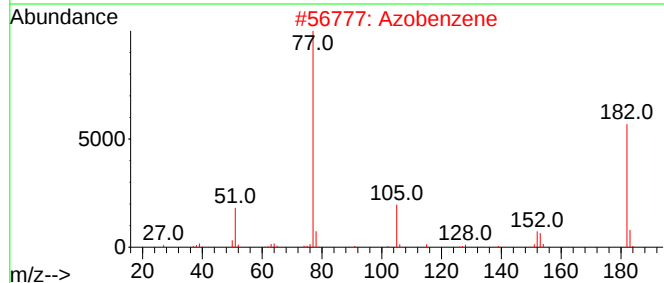
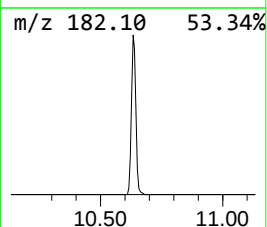
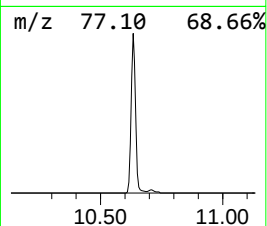
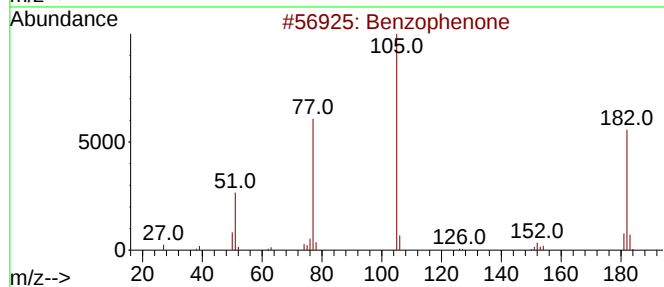
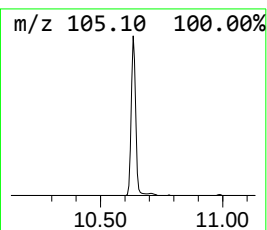
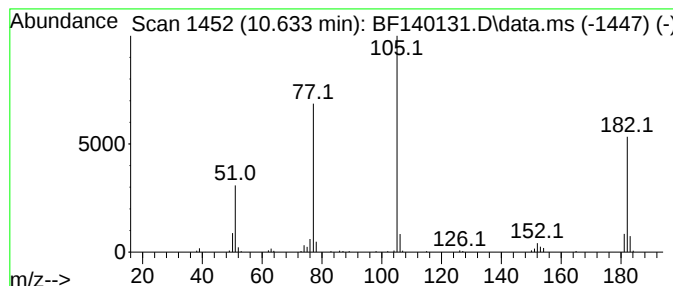
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Peak Number 2 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.633	2.86 ng	146155	Acenaphthene-d10	9.922

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Azobenzene	182	C12H10N2	000103-33-3	64
3			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	53
4			1,2-Propanedione, 1-phenyl-	148	C9H8O2	000579-07-7	47
5			Disulfide, dibenzoyl	274	C14H10O2S2	000644-32-6	47



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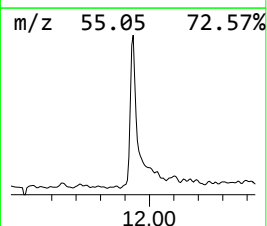
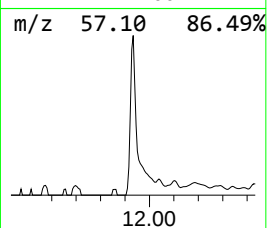
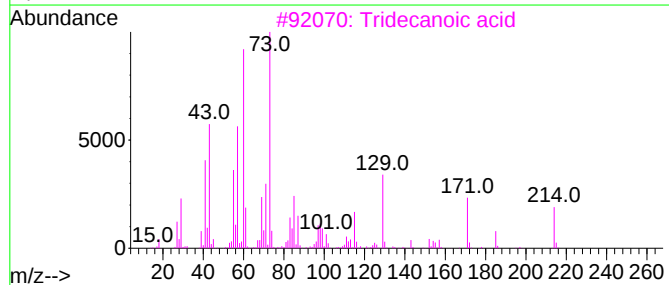
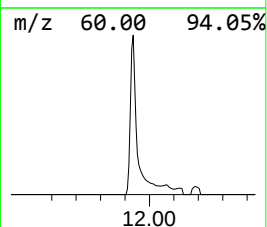
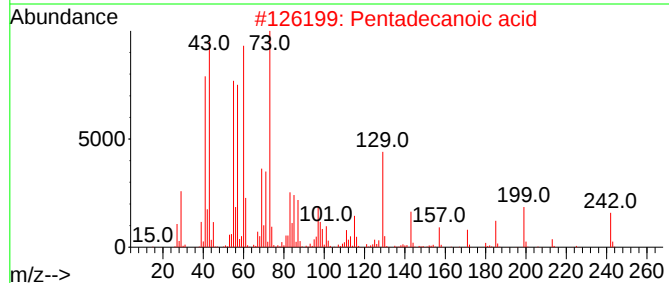
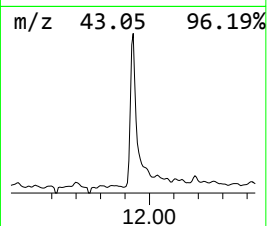
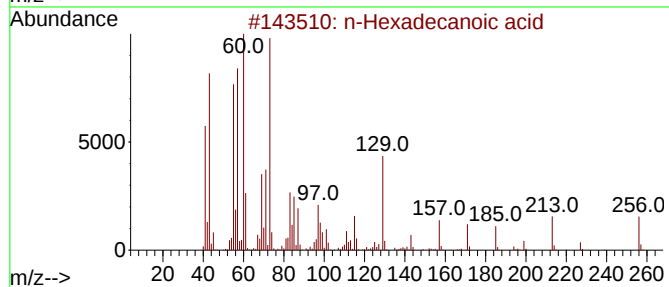
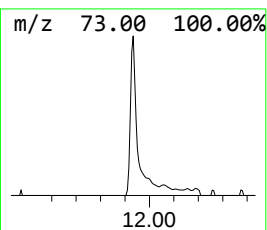
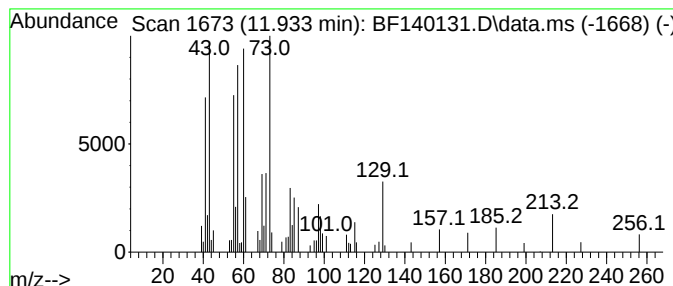
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.933	2.50 ng	100848	Phenanthrene-d10	11.410

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			Tridecanoic acid	214	C13H26O2	000638-53-9	86
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5			n-Decanoic acid	172	C10H20O2	000334-48-5	50



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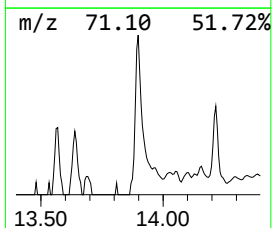
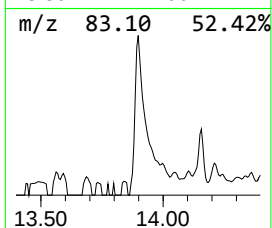
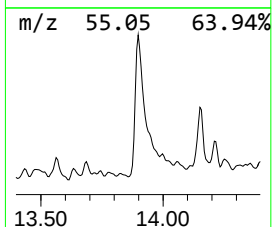
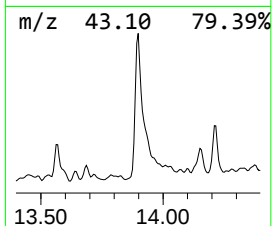
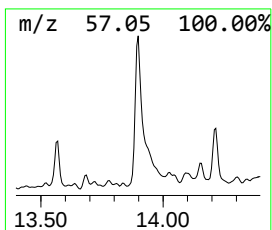
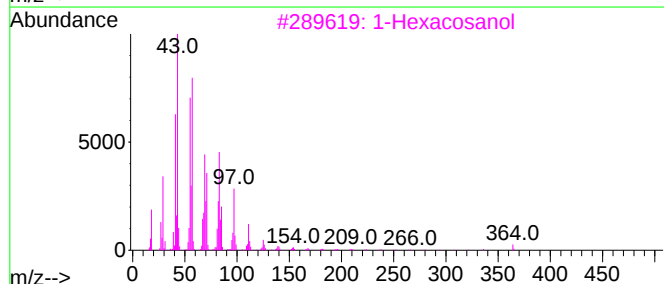
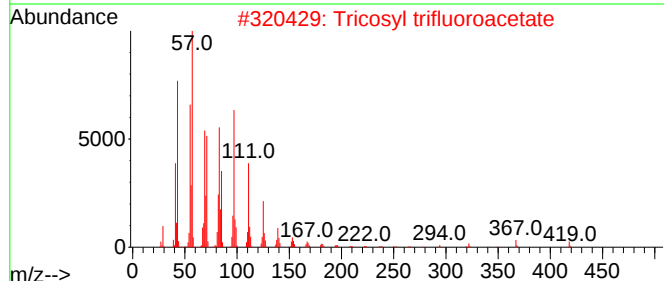
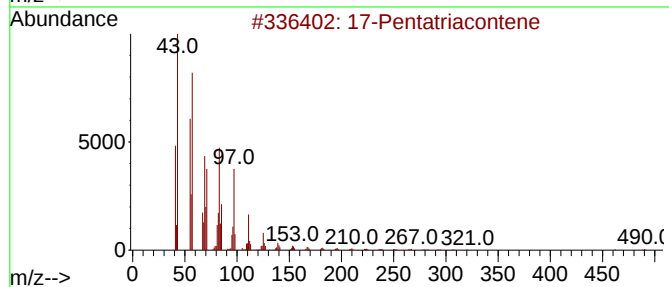
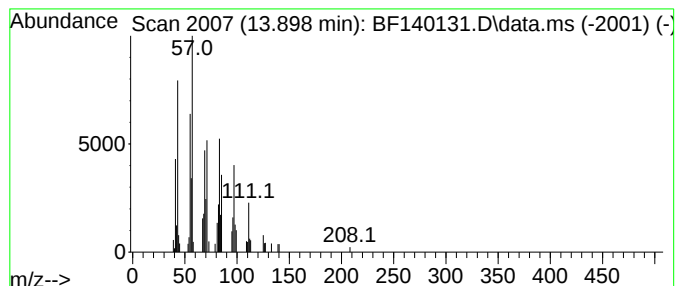
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Peak Number 4 17-Pentatriacontene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.898	2.66 ng	93786	Chrysene-d12	14.051

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			17-Pentatriacontene	491	C35H70	006971-40-0	91
2			Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	91
3			1-Hexacosanol	382	C26H54O	000506-52-5	90
4			Oxirane, [(dodecyloxy)methyl]-	242	C15H30O2	002461-18-9	87
5			Butyl hexadecyl ether	298	C20H42O	1010406-40-5	83



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.187	37.4	ng	1458670	1	6.886	780761	20.0
Benzophenone	10.633	2.9	ng	146155	3	9.922	1021680	20.0
n-Hexadecanoic ...	11.933	2.5	ng	100848	4	11.410	807238	20.0
17-Pentatriacon...	13.898	2.7	ng	93786	5	14.051	705638	20.0