

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102124\
 Data File : BF139895.D
 Acq On : 21 Oct 2024 11:27
 Operator : RC/JU
 Sample : P4425-07
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-4

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: BF139895.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	8	16	28	rVB	1855538	3005482	96.50%	11.195%
2	5.110	505	513	520	rVB	187689	285904	9.18%	1.065%
3	5.504	573	580	585	rBV	2012309	2732817	87.75%	10.179%
4	6.504	743	750	755	rBV	2099635	2902704	93.20%	10.812%
5	6.887	810	815	821	rVB	832590	1052594	33.80%	3.921%
6	6.945	821	825	830	rBV	28466	34720	1.11%	0.129%
7	7.445	904	910	915	rBV	1426056	1810623	58.14%	6.744%
8	7.698	948	953	958	rBV	104168	123495	3.97%	0.460%
9	8.169	1027	1033	1038	rBV	1108160	1375655	44.17%	5.124%
10	8.381	1061	1069	1082	rVB	31584	43985	1.41%	0.164%
11	9.245	1210	1216	1221	rBV	2465143	3114486	100.00%	11.601%
12	9.927	1326	1332	1337	rBV	1199452	1535228	49.29%	5.719%
13	10.639	1447	1453	1460	rBV	555482	707519	22.72%	2.635%
14	10.710	1460	1465	1477	rBV	1389245	1745337	56.04%	6.501%
15	11.410	1579	1584	1591	rBV	1171343	1458002	46.81%	5.431%
16	11.474	1591	1595	1599	rVB2	30593	38791	1.25%	0.144%
17	11.933	1665	1673	1688	rBV2	212780	356698	11.45%	1.329%
18	12.716	1801	1806	1820	rBV	55364	103863	3.33%	0.387%
19	12.998	1848	1854	1859	rBV	1947372	2468328	79.25%	9.194%
20	13.892	2001	2006	2027	rBV	103348	195183	6.27%	0.727%
21	14.051	2027	2033	2040	rBV	633353	831106	26.69%	3.096%
22	15.527	2278	2284	2291	rBV	598546	924086	29.67%	3.442%

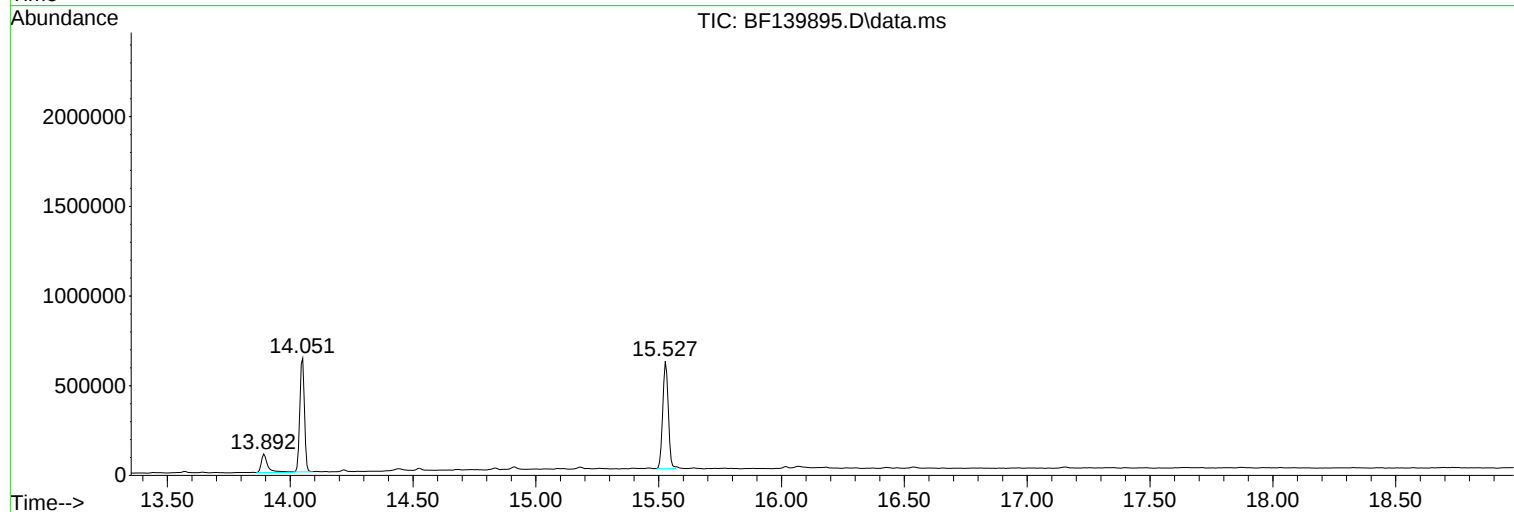
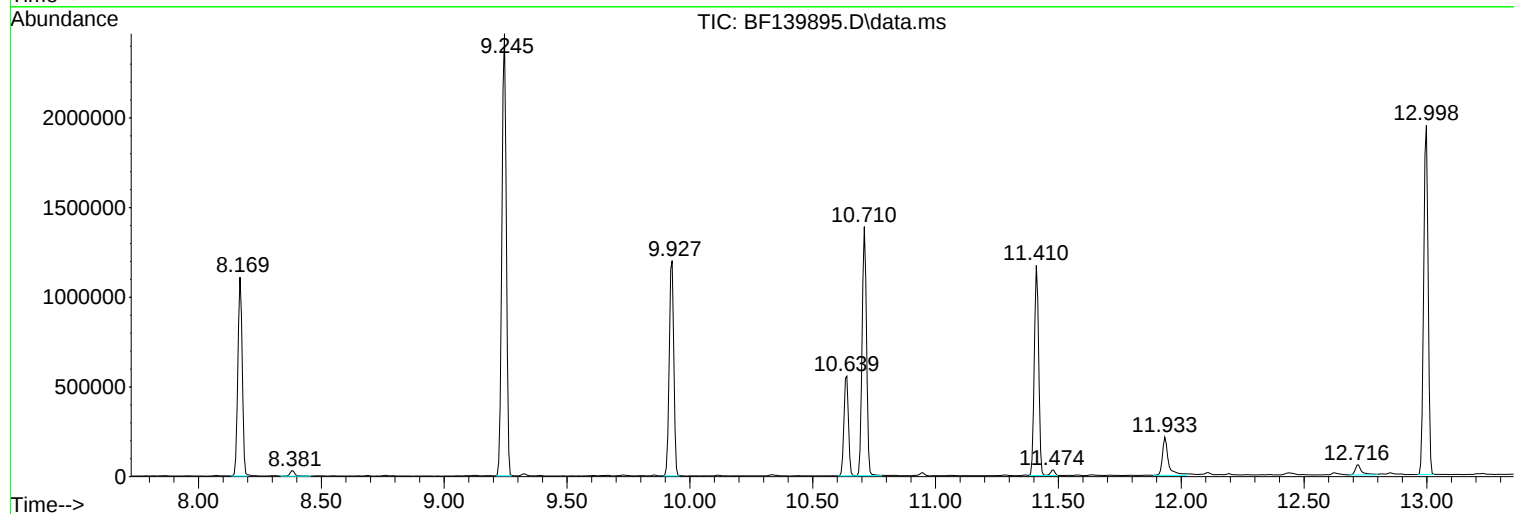
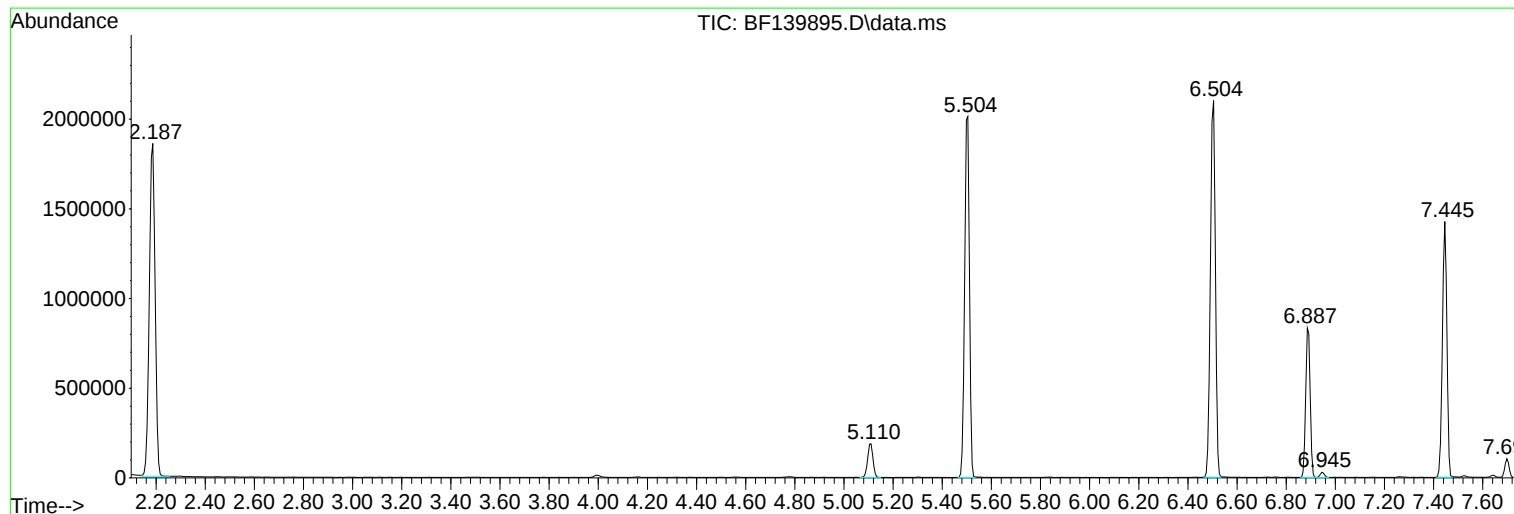
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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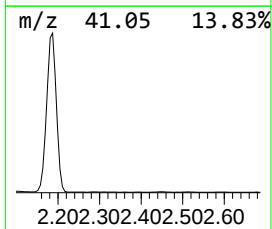
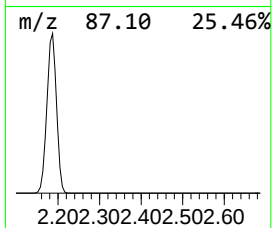
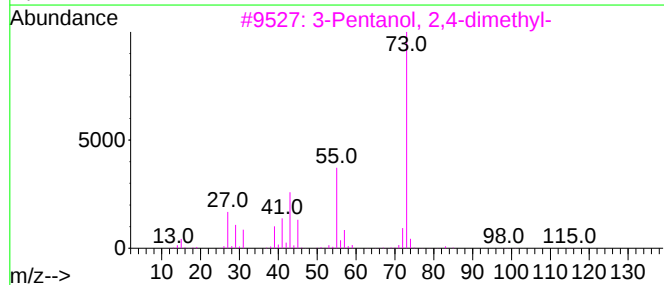
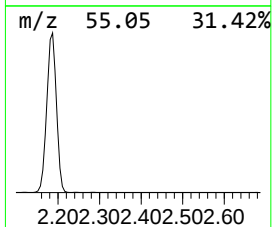
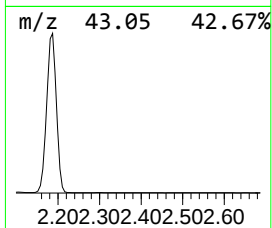
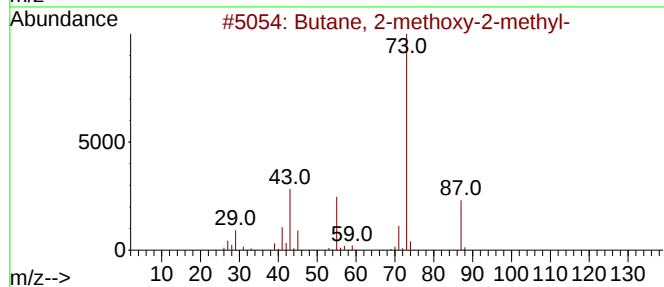
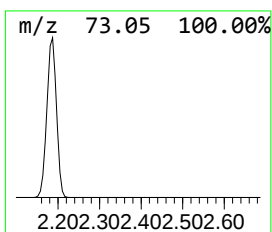
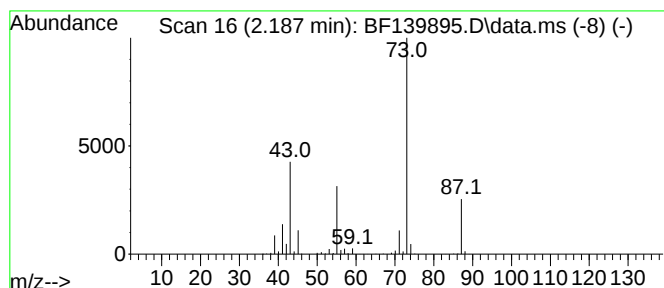
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.187	57.11 ng	3005480	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			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5			Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	17



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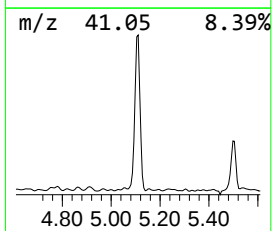
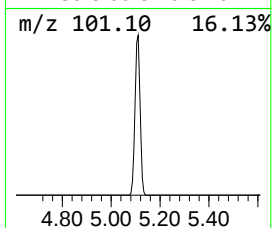
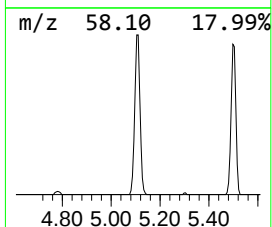
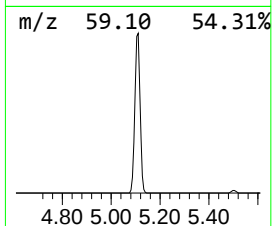
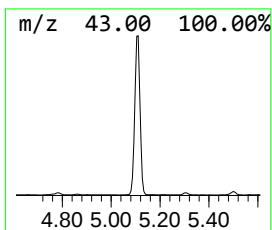
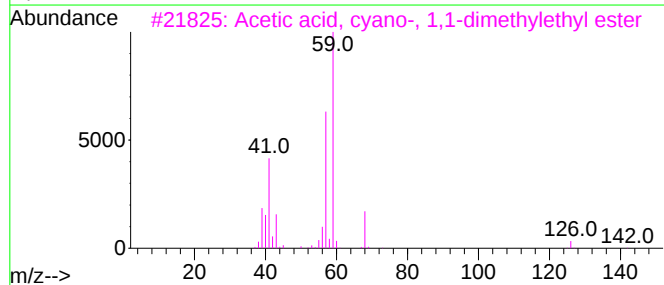
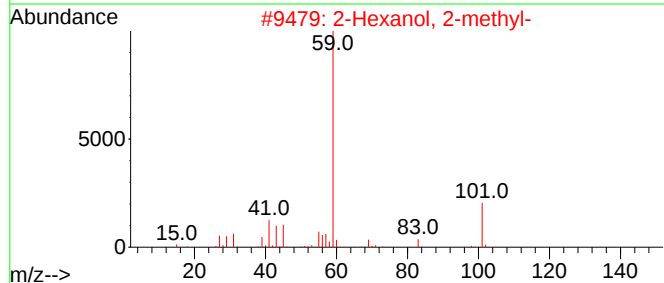
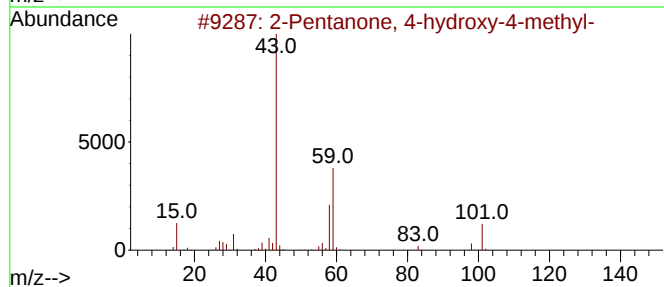
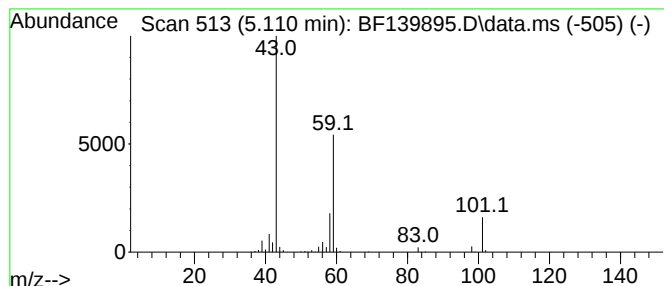
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.110	5.43 ng	285904	1,4-Dichlorobenzene-d4	6.886

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	17
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16



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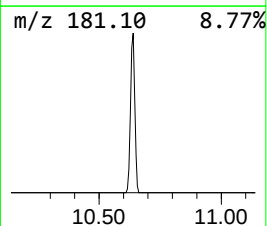
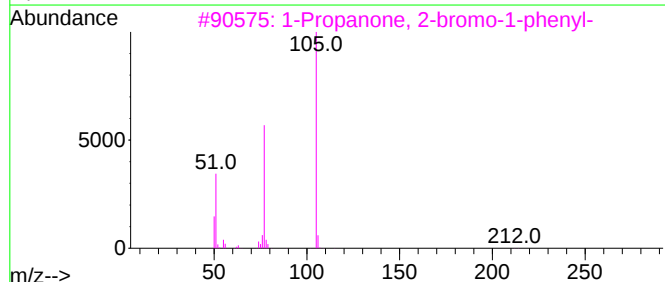
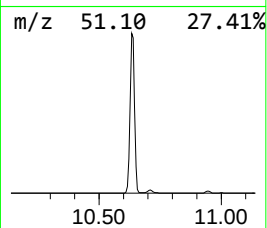
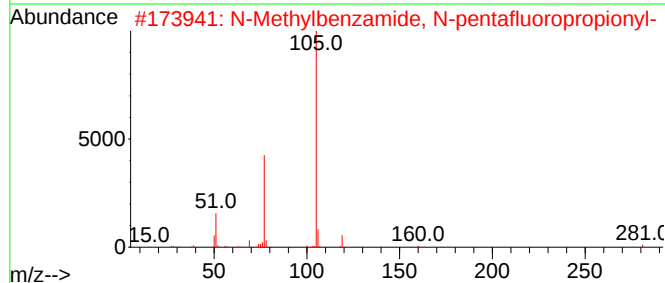
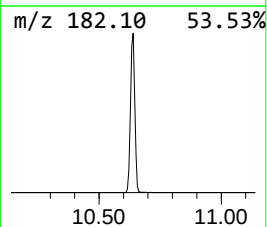
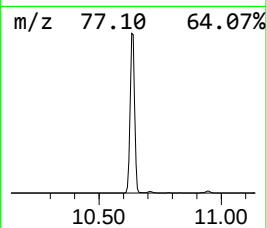
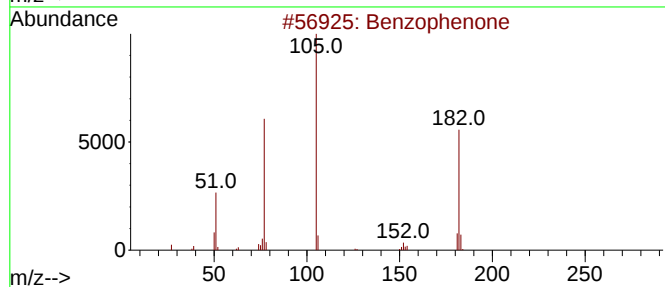
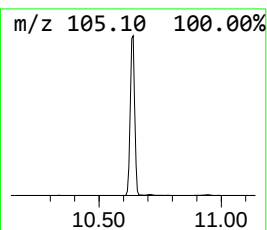
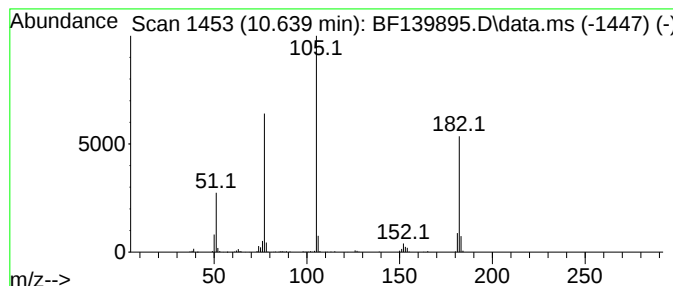
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Peak Number 3 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.639	9.22 ng	707519	Acenaphthene-d10	9.927

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			N-Methylbenzamide, N-pentafluoro...	281	C11H8F5NO2	1000446-98-1	47
3			1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47
4			Vinyl benzoate	148	C9H8O2	000769-78-8	47
5			Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	47



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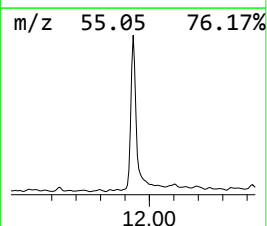
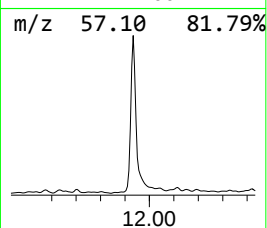
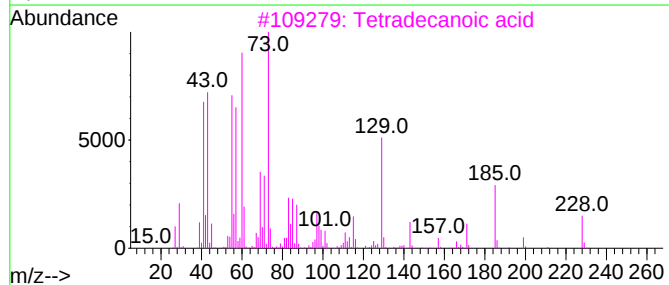
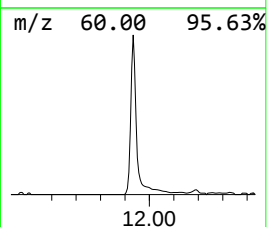
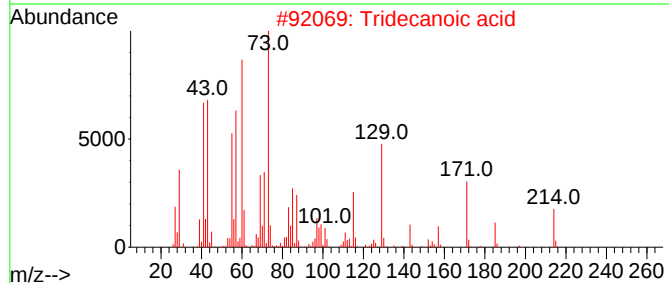
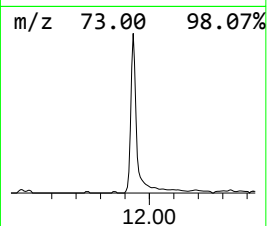
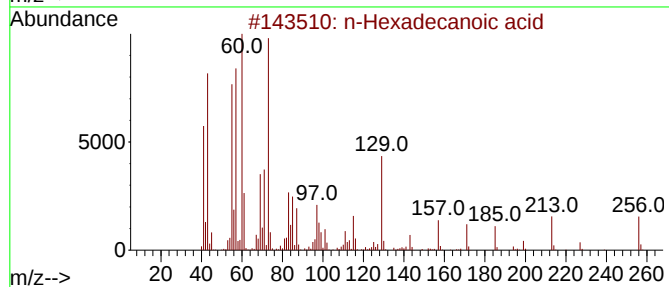
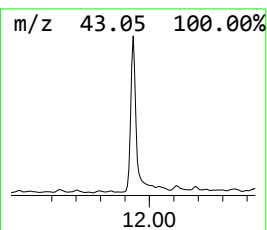
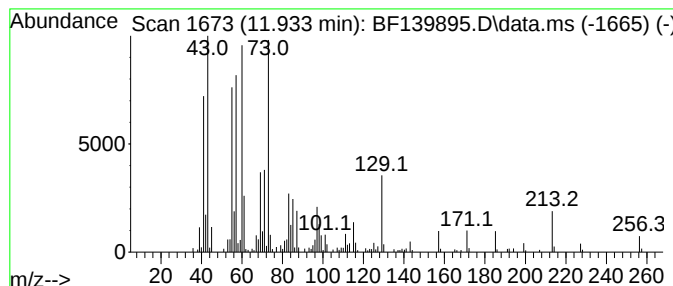
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.933	4.89 ng	356698	Phenanthrene-d10	11.410

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	93
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	91
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
5			n-Decanoic acid	172	C10H20O2	000334-48-5	68



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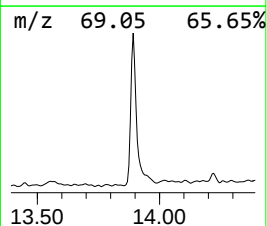
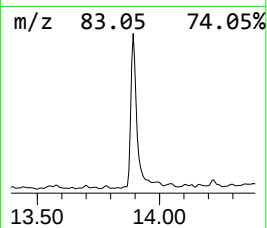
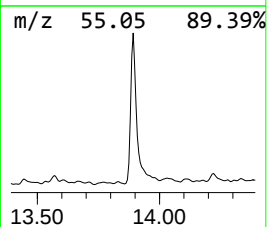
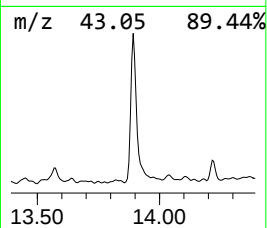
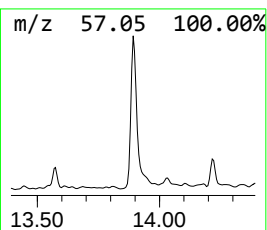
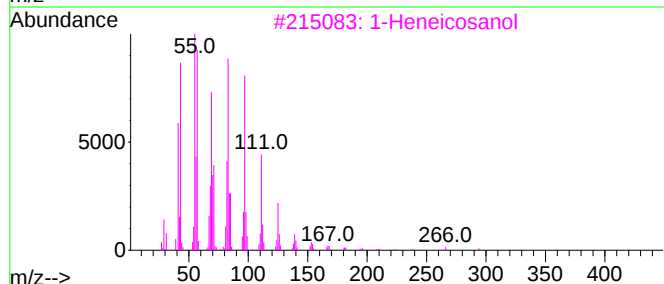
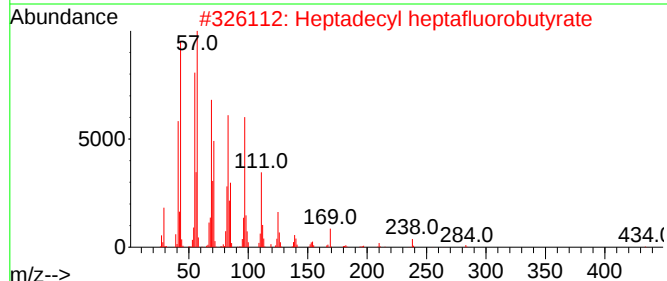
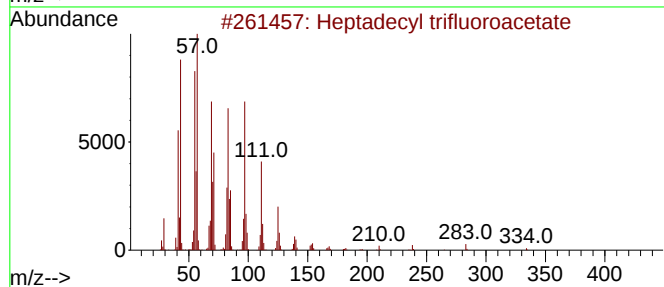
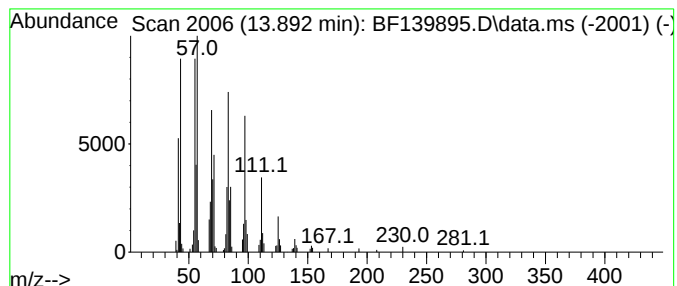
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Peak Number 5 Heptadecyl trifluoroacetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.892	4.70 ng	195183	Chrysene-d12	14.051

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	94
2			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	93
3			1-Heneicosanol	312	C21H44O	015594-90-8	93
4			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
5			Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.187	57.1	ng	3005480	1	6.886	1052590	20.0
2-Pentanone, 4-...	5.110	5.4	ng	285904	1	6.886	1052590	20.0
Benzophenone	10.639	9.2	ng	707519	3	9.927	1535230	20.0
n-Hexadecanoic ...	11.933	4.9	ng	356698	4	11.410	1458000	20.0
Heptadecyl trif...	13.892	4.7	ng	195183	5	14.051	831106	20.0