

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101824\
 Data File : BF139862.D
 Acq On : 18 Oct 2024 19:09
 Operator : RC/JU
 Sample : P4425-09
 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: BF139862.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.169	5	13	26	rVB	1686655	2666403	100.00%	14.250%
2	5.098	505	511	521	rVB	142483	212453	7.97%	1.135%
3	5.498	573	579	584	rBV	1768754	2255013	84.57%	12.052%
4	6.498	743	749	764	rVB	1677532	2245347	84.21%	12.000%
5	6.887	810	815	821	rBV	578134	730339	27.39%	3.903%
6	7.445	904	910	915	rBV	1048838	1281701	48.07%	6.850%
7	7.698	948	953	958	rBV	71116	83156	3.12%	0.444%
8	8.169	1028	1033	1038	rBV	679911	822752	30.86%	4.397%
9	8.381	1064	1069	1077	rVB	22455	28458	1.07%	0.152%
10	9.245	1210	1216	1221	rBV	1576953	1924931	72.19%	10.288%
11	9.922	1326	1331	1336	rBV	583465	729937	27.38%	3.901%
12	10.633	1447	1452	1460	rVB	142434	173301	6.50%	0.926%
13	10.710	1460	1465	1477	rBV	789169	999214	37.47%	5.340%
14	11.410	1579	1584	1589	rBV	628946	760019	28.50%	4.062%
15	11.927	1668	1672	1684	rBV2	34973	58101	2.18%	0.311%
16	12.998	1848	1854	1859	rBV	1693147	2200228	82.52%	11.759%
17	13.574	1945	1952	1960	rBV3	11729	27513	1.03%	0.147%
18	13.892	2001	2006	2017	rBV	92469	176807	6.63%	0.945%
19	14.051	2027	2033	2040	rBV	588904	781696	29.32%	4.178%
20	14.527	2110	2114	2119	rBV3	15753	27480	1.03%	0.147%
21	14.910	2176	2179	2184	rBV	20042	26768	1.00%	0.143%
22	15.527	2278	2284	2290	rBV	319073	499728	18.74%	2.671%

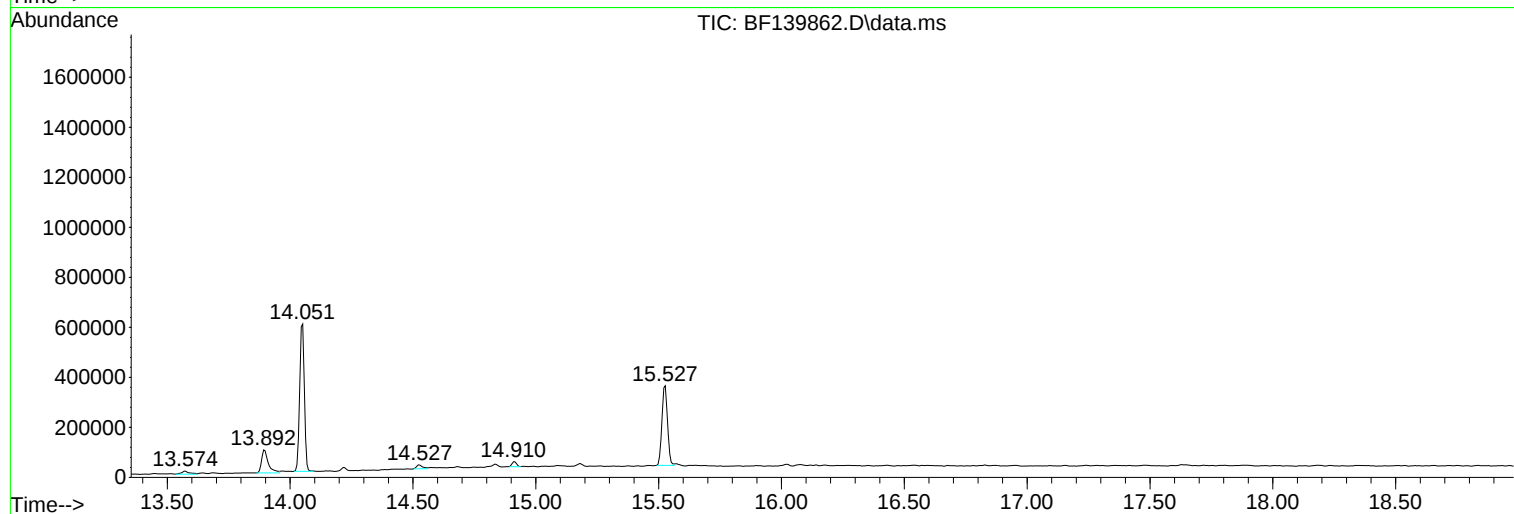
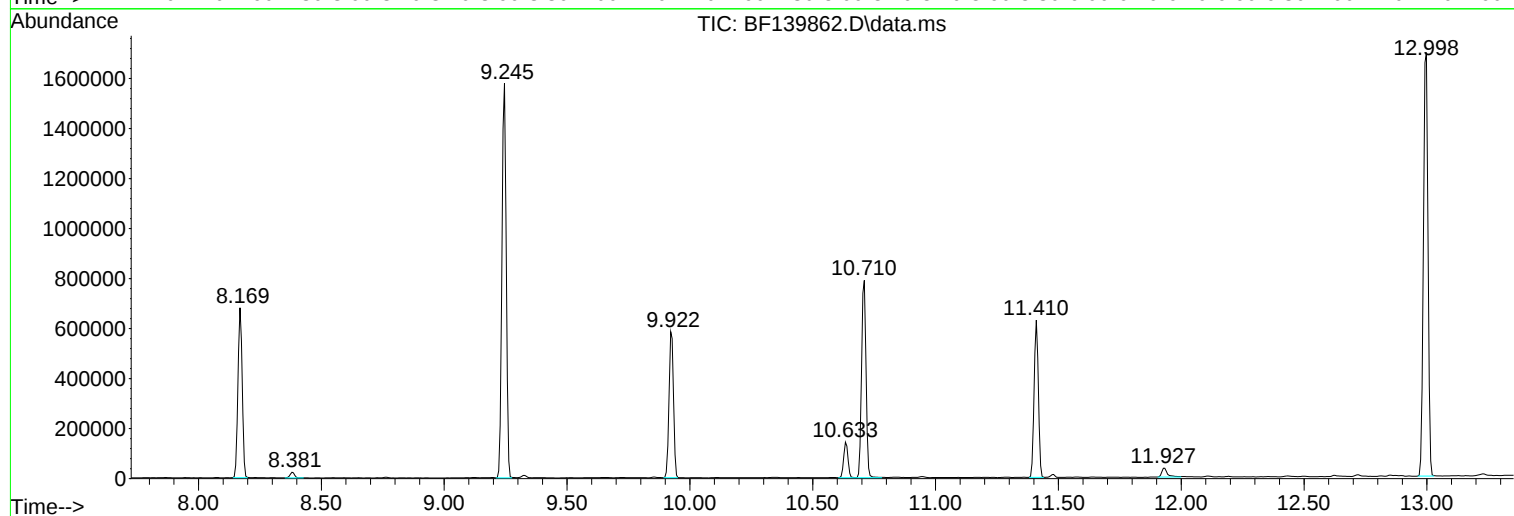
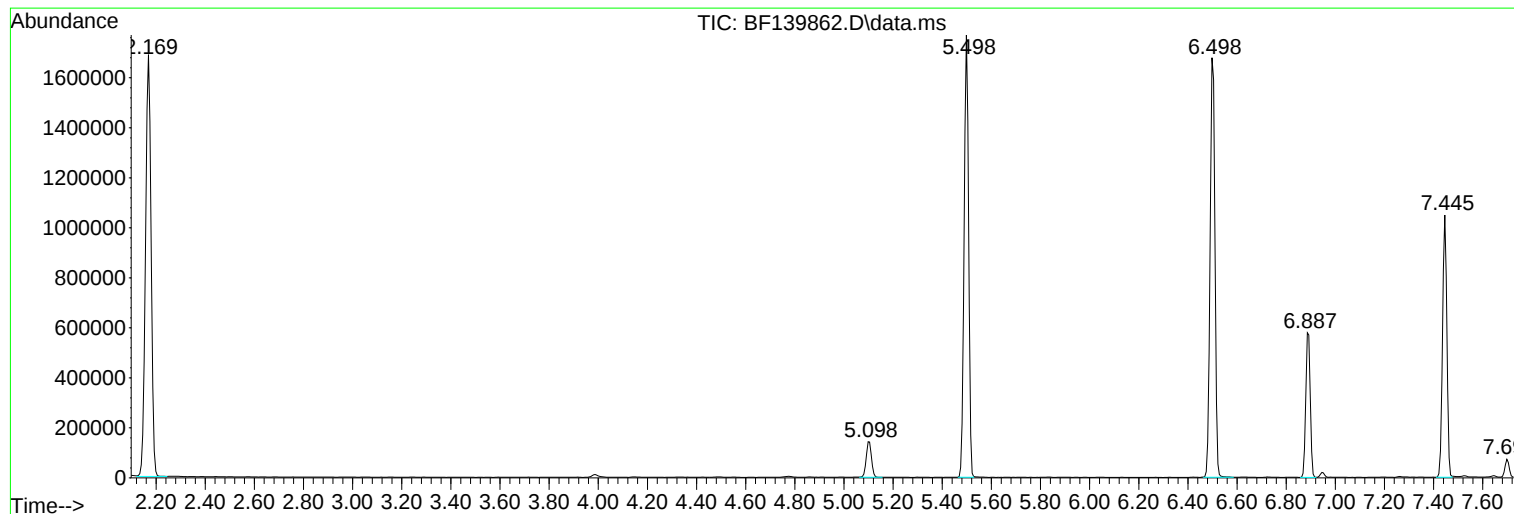
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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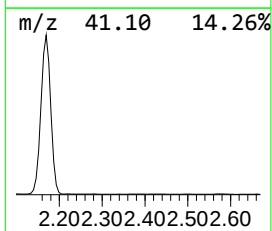
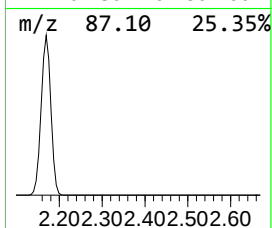
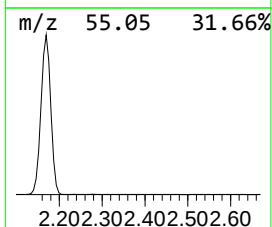
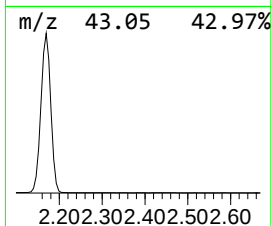
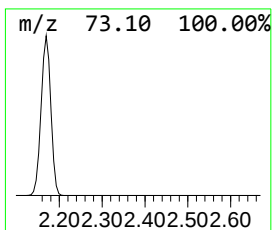
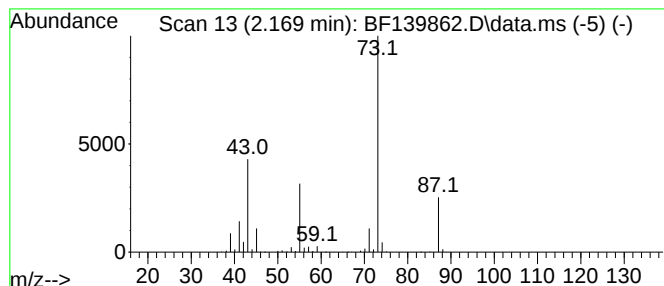
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.169	73.02 ng	2666400	1,4-Dichlorobenzene-d4	6.892

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			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5			Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9



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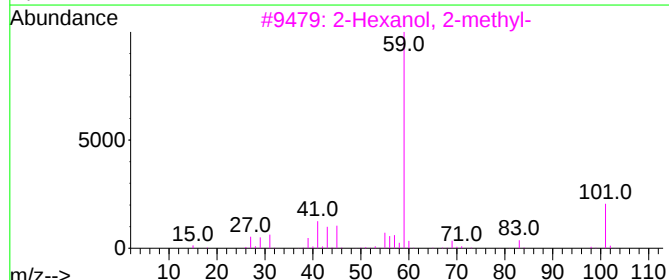
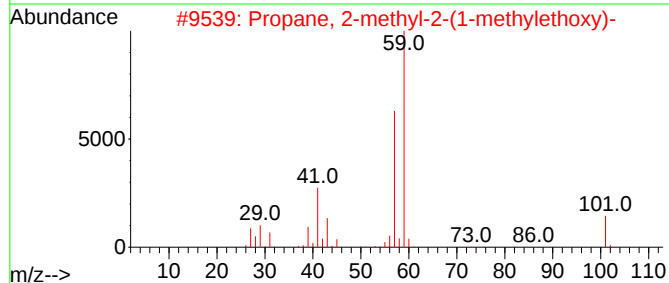
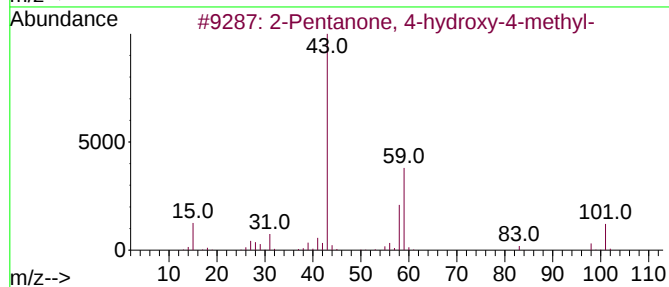
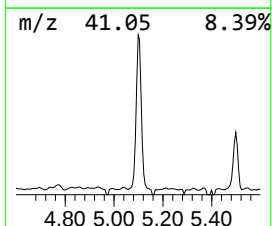
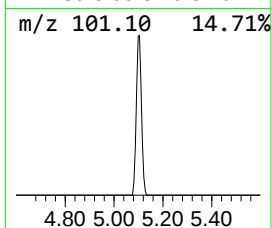
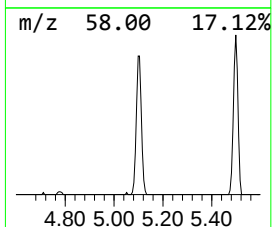
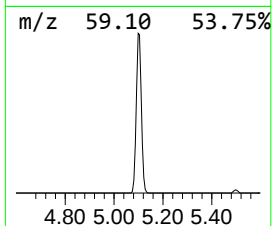
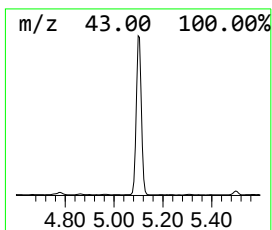
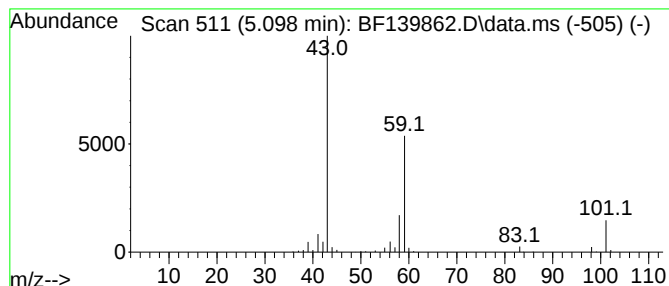
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD			R.T.
5.098	5.82 ng	212453	1,4-Dichlorobenzene-d4			6.892
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-		116	C6H12O2	000123-42-2	59
2	Propane, 2-methyl-2-(1-methyleth...		116	C7H16O	017348-59-3	42
3	2-Hexanol, 2-methyl-		116	C7H16O	000625-23-0	40
4	3-Hexanol, 4-methyl-		116	C7H16O	000615-29-2	33
5	3-Octanol		130	C8H18O	000589-98-0	33



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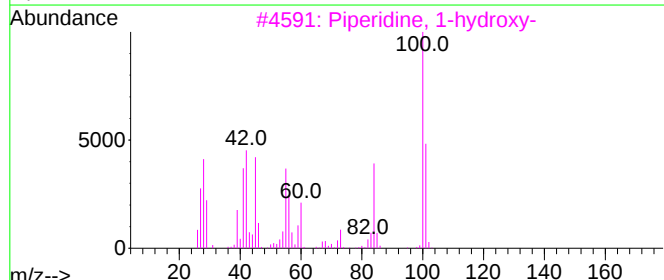
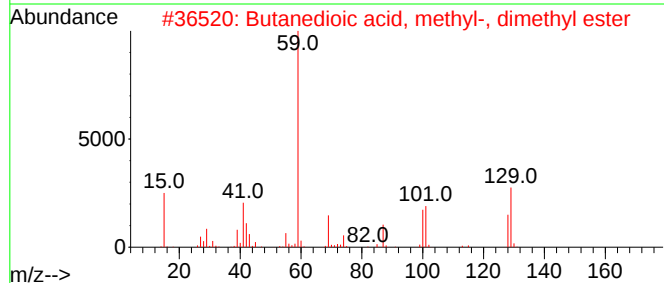
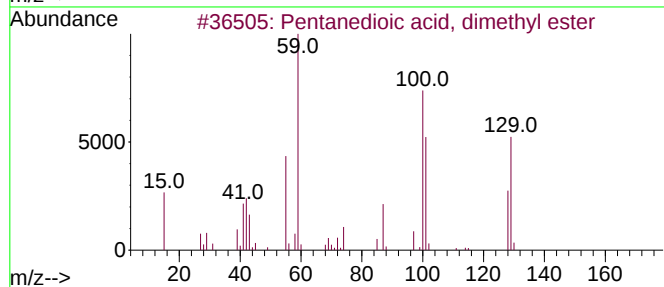
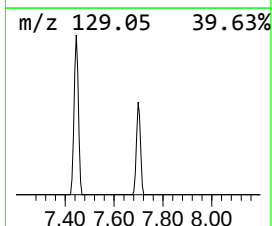
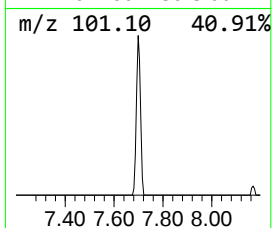
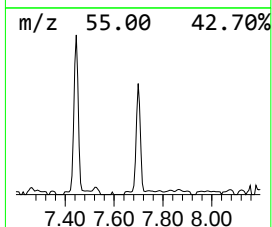
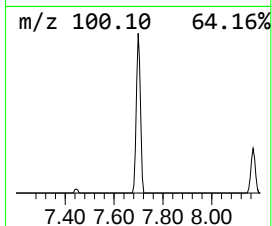
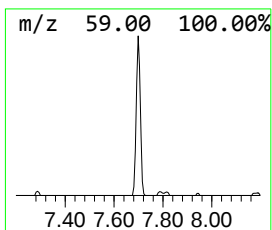
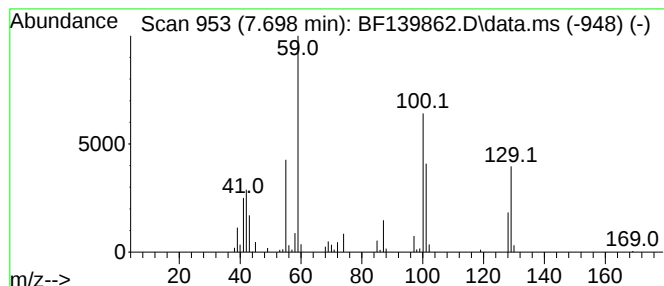
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Peak Number 3 Pentanedioic acid, dimethyl... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.698	2.02 ng	83156	Naphthalene-d8	8.169

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentanedioic acid, dimethyl ester	160	C7H12O4	001119-40-0	91
2			Butanedioic acid, methyl-, dimet...	160	C7H12O4	001604-11-1	45
3			Piperidine, 1-hydroxy-	101	C5H11NO	004801-58-5	38
4			Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	37
5			Propane-1,2,3-triamine	89	C3H11N3	021291-99-6	12



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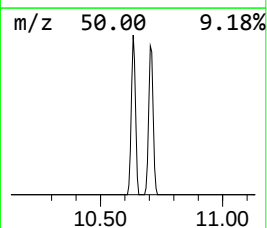
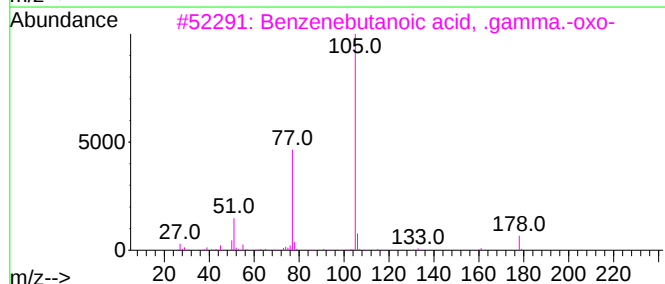
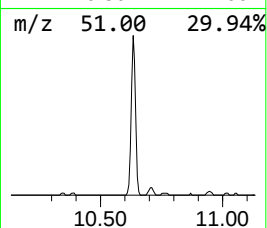
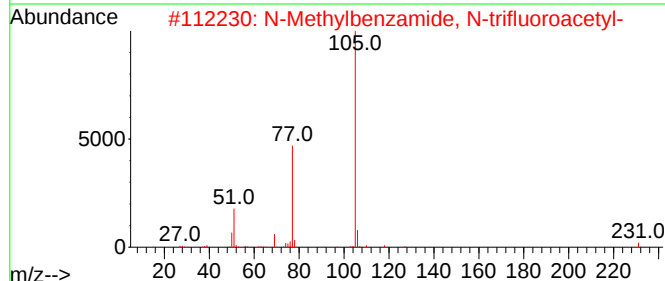
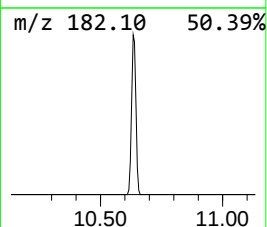
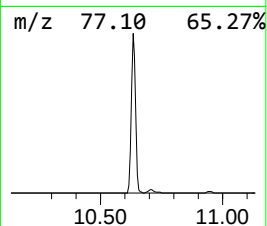
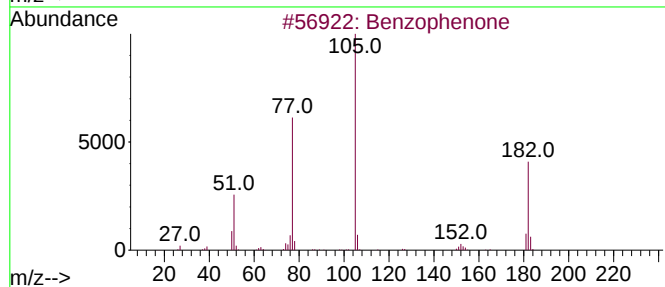
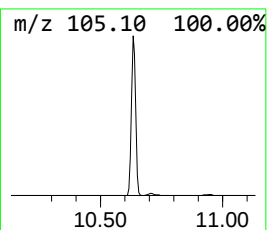
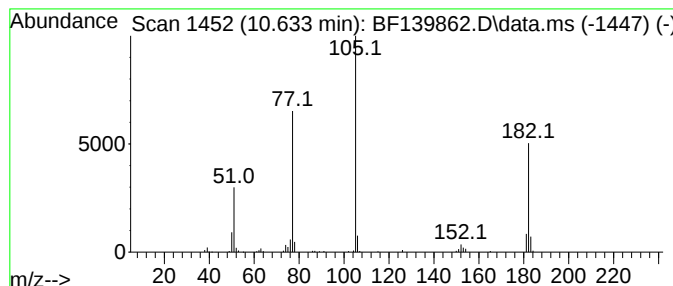
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Peak Number 4 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.633	4.75 ng	173301	Acenaphthene-d10	9.922

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			N-Methylbenzamide, N-trifluoroac...	231	C10H8F3NO2	1000446-91-5	50
3			Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	50
4			Pentafluoroethyl phenyl ketone	224	C9H5F5O	000394-52-5	50
5			Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	50



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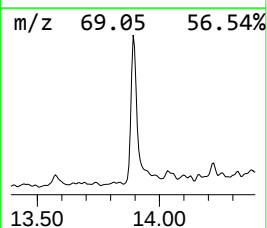
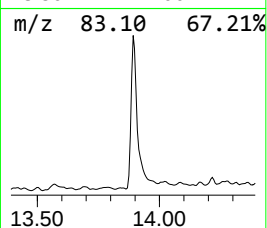
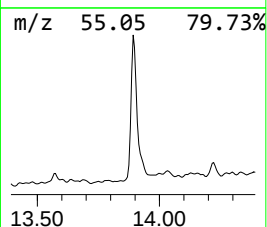
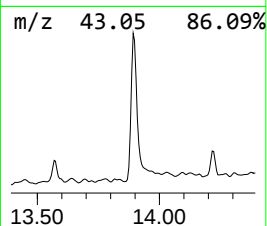
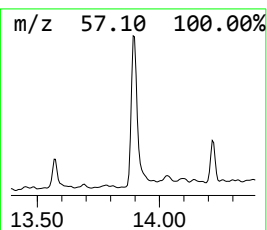
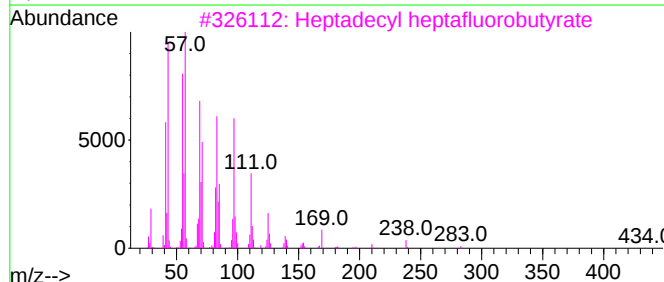
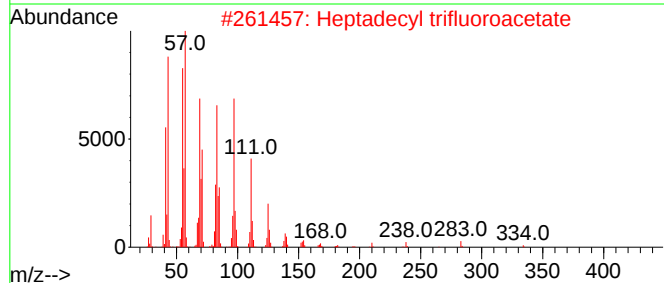
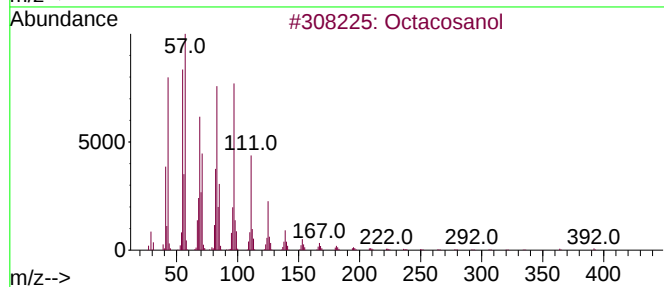
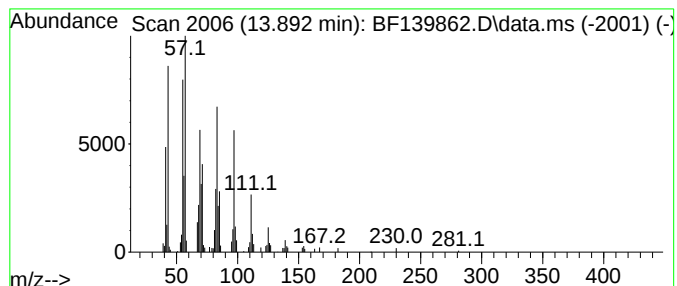
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Peak Number 5 Octacosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.892	4.52 ng	176807	Chrysene-d12	14.051

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosanol	410	C28H58O	000557-61-9	94
2			Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	94
3			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
4			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
5			Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	94



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.169	73.0	ng	2666400	1	6.892	730339	20.0
2-Pentanone, 4-...	5.098	5.8	ng	212453	1	6.892	730339	20.0
Pentanedioic ac...	7.698	2.0	ng	83156	2	8.169	822752	20.0
Benzophenone	10.633	4.8	ng	173301	3	9.922	729937	20.0
Octacosanol	13.892	4.5	ng	176807	5	14.051	781696	20.0