

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030524\
 Data File : BF137507.D
 Acq On : 05 Mar 2024 18:35
 Operator : CG\JU
 Sample : P1672-01
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-1

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-BF022924.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF137507.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.199	15	19	28	rVB	27368	46322	1.51%	0.177%
2	3.416	224	226	244	rBV	80071	224549	7.33%	0.856%
3	5.087	507	510	520	rVB	40409	56690	1.85%	0.216%
4	5.487	575	578	600	rBV	2859248	2905864	94.89%	11.076%
5	6.481	744	747	769	rBV	2889699	3062478	100.00%	11.672%
6	6.845	806	809	818	rBV	1023803	874291	28.55%	3.332%
7	7.404	901	904	917	rBV	2046789	1803030	58.87%	6.872%
8	8.122	1022	1026	1045	rBV	1343483	1173630	38.32%	4.473%
9	8.445	1078	1081	1089	rBV	51871	95381	3.11%	0.364%
10	9.198	1206	1209	1221	rBV	3679147	3000355	97.97%	11.436%
11	9.875	1321	1324	1338	rBV	1384339	1299936	42.45%	4.955%
12	9.986	1338	1343	1357	rVV	2438449	3051945	99.66%	11.632%
13	10.669	1456	1459	1474	rBV	1638877	1560692	50.96%	5.948%
14	10.792	1477	1480	1493	rVB	126943	186345	6.08%	0.710%
15	11.375	1575	1579	1582	rBV	1305217	1238451	40.44%	4.720%
16	11.780	1644	1648	1654	rBV	46636	43348	1.42%	0.165%
17	12.492	1762	1769	1772	rBV5	62912	72927	2.38%	0.278%
18	12.592	1781	1786	1792	rBV	146054	160371	5.24%	0.611%
19	12.822	1820	1825	1829	rBV	143799	155287	5.07%	0.592%
20	12.974	1847	1851	1860	rBV	2797758	2544021	83.07%	9.696%
21	13.469	1931	1935	1939	rBV2	40323	55172	1.80%	0.210%
22	13.563	1947	1951	1953	rBV	37652	36525	1.19%	0.139%
23	13.892	2004	2007	2018	rBV2	108937	167993	5.49%	0.640%
24	14.033	2024	2031	2035	rBV	911510	983666	32.12%	3.749%
25	14.216	2059	2062	2066	rVB	42840	41213	1.35%	0.157%
26	14.521	2111	2114	2117	rBV	52923	52071	1.70%	0.198%
27	14.851	2167	2170	2176	rVB2	38049	49044	1.60%	0.187%
28	15.104	2210	2213	2224	rBV	67298	150217	4.91%	0.573%
29	15.215	2228	2232	2236	rVB3	42253	53706	1.75%	0.205%
30	15.421	2264	2267	2273	rVB	43428	56404	1.84%	0.215%
31	15.492	2275	2279	2284	rBV	63251	92788	3.03%	0.354%
32	15.557	2285	2290	2299	rVV	687934	942020	30.76%	3.590%

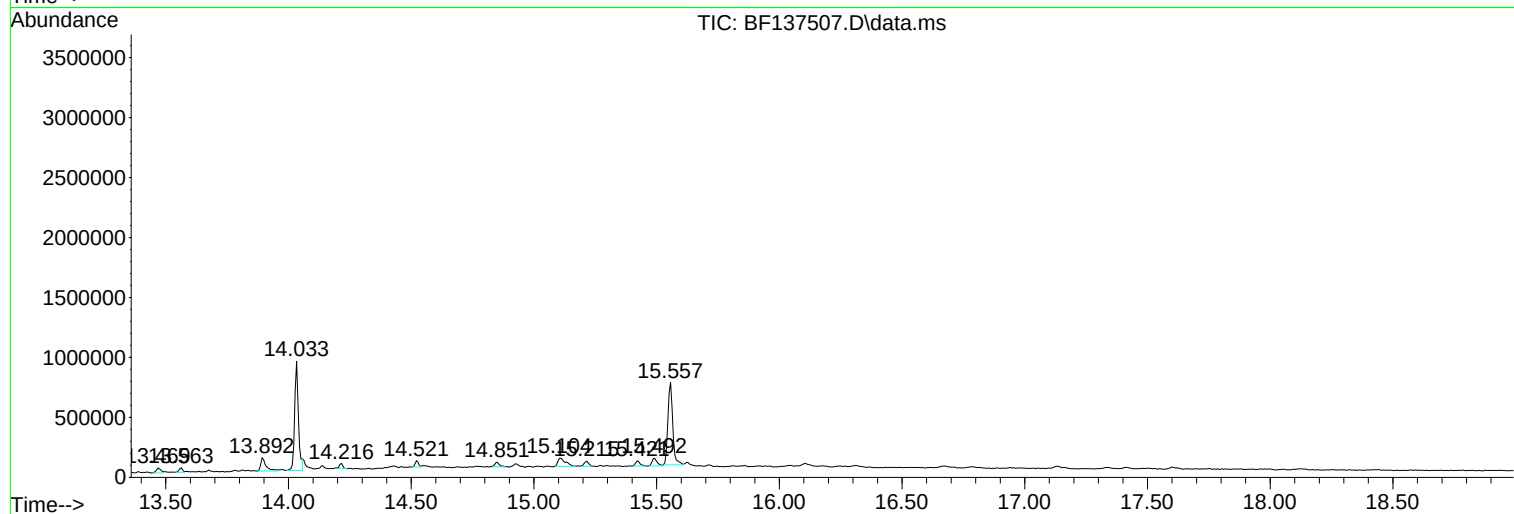
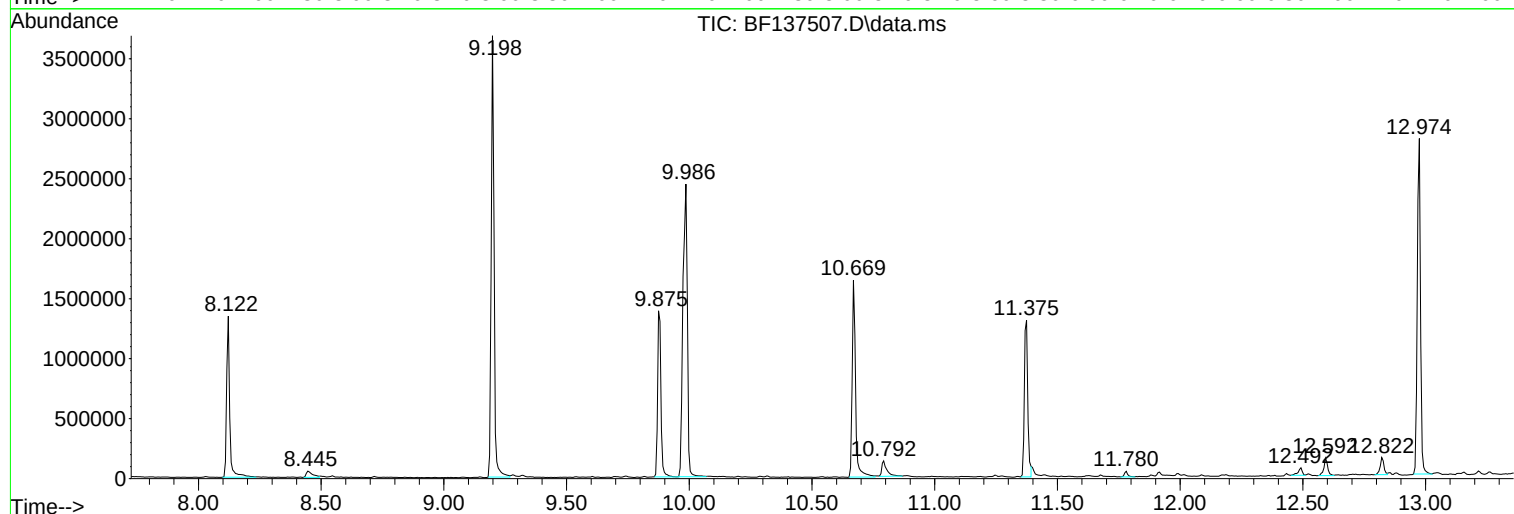
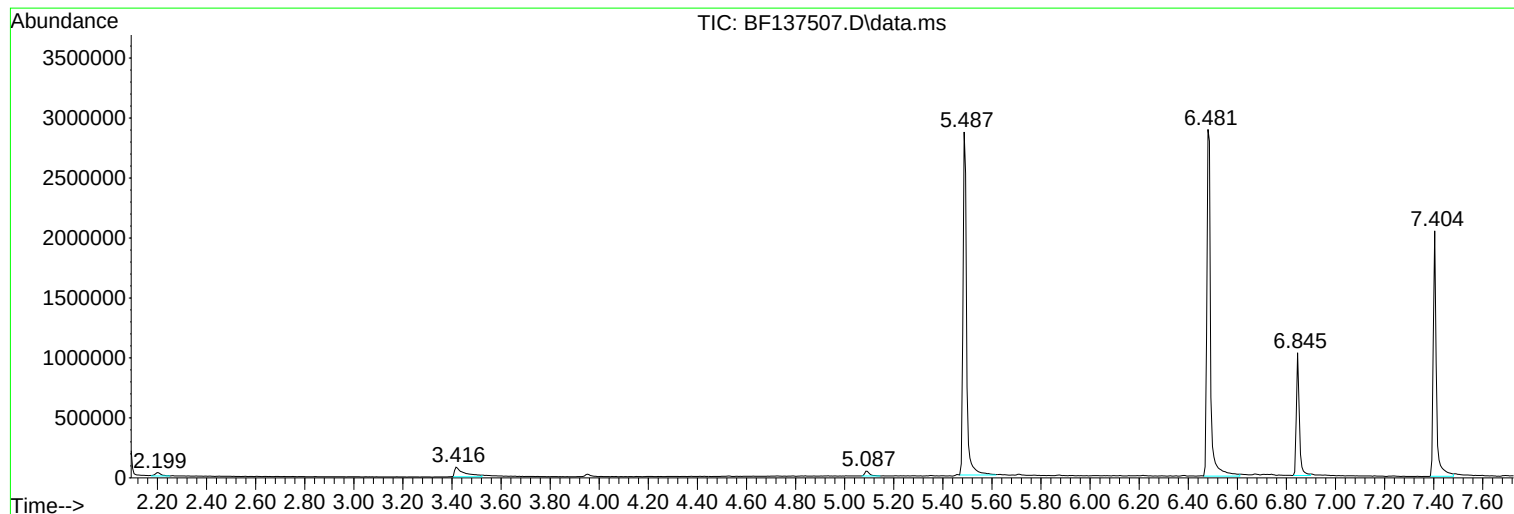
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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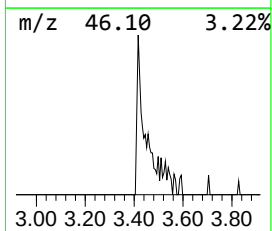
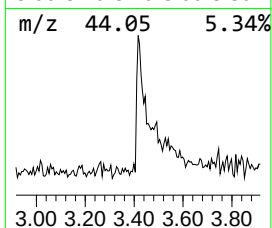
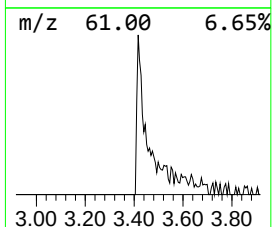
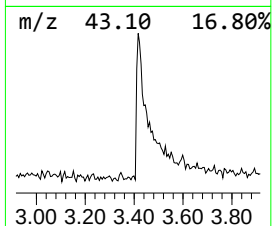
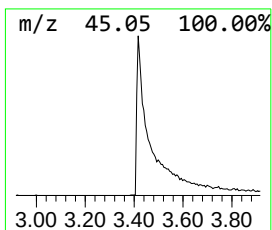
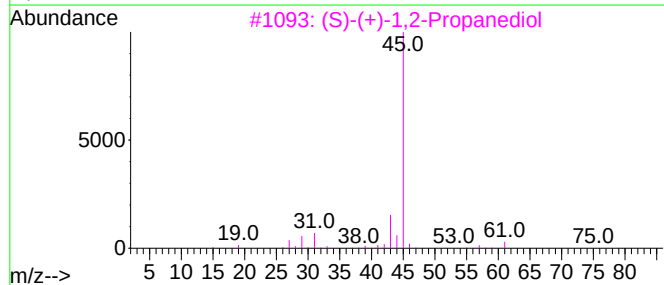
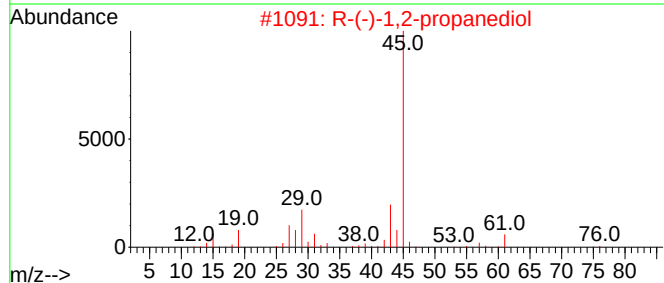
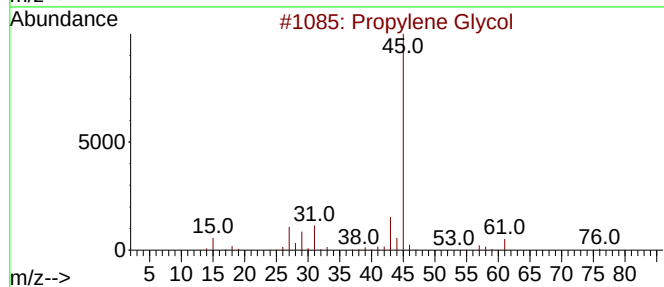
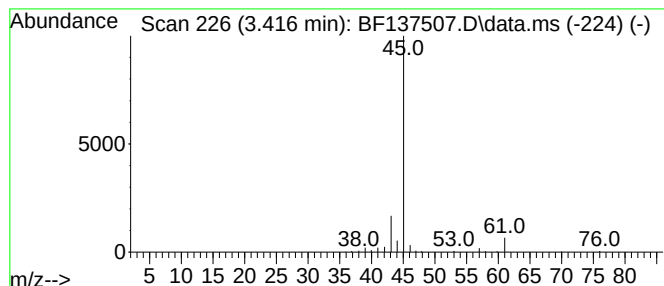
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Propylene Glycol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.416	5.14 ng	224549	1,4-Dichlorobenzene-d4	6.845

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propylene Glycol	76	C3H8O2	000057-55-6	78
2			R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	78
3			(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	40
4			Isopropyl Alcohol	60	C3H8O	000067-63-0	9
5			Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	9



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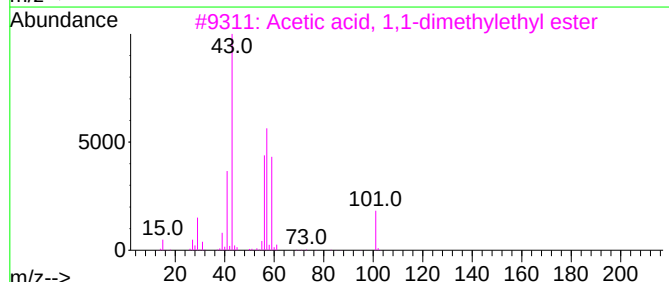
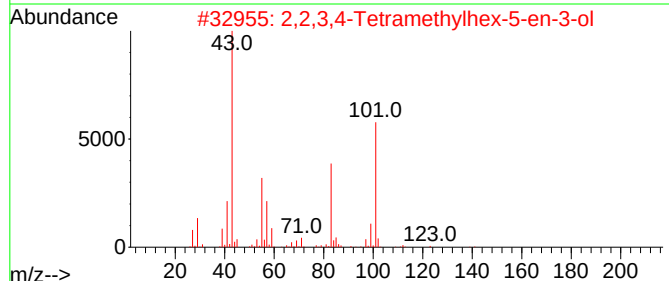
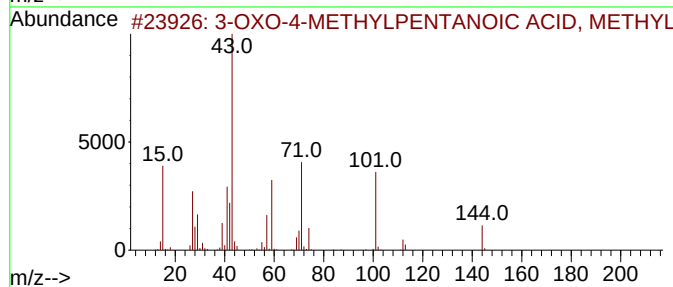
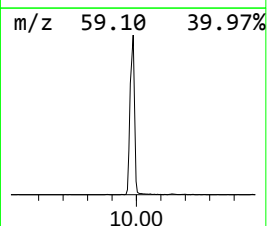
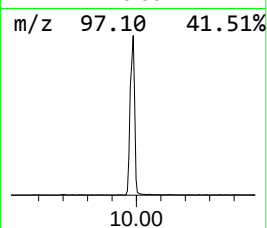
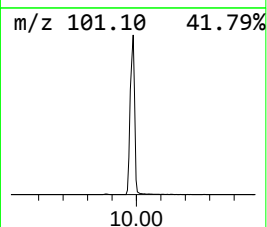
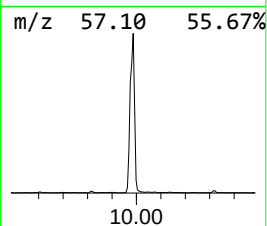
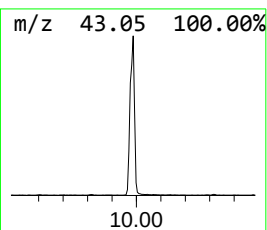
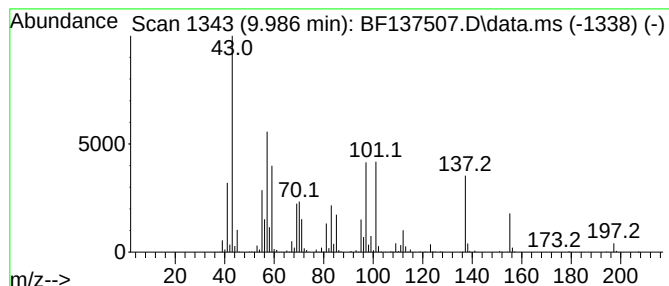
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Peak Number 2 unknown9.986 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.986	46.96 ng	3051950	Acenaphthene-d10	9.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-OXO-4-METHYLPENTANOIC ACID, ME...	144	C7H12O3	042558-54-3	16
2			2,2,3,4-Tetramethylhex-5-en-3-ol	156	C10H20O	1010191-06-9	14
3			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	12
4			Carbonic acid, prop-1-en-2-yl un...	256	C15H28O3	1000382-90-6	12
5			11-Tricosene	322	C23H46	052078-56-5	12



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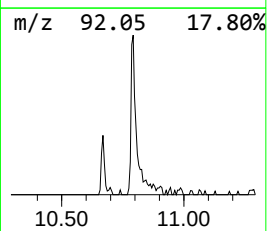
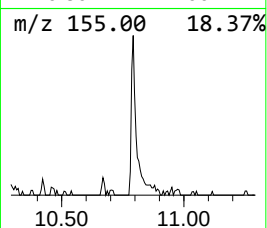
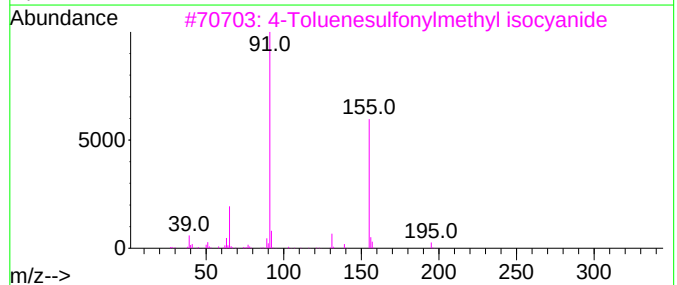
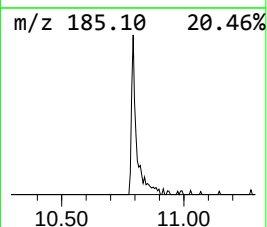
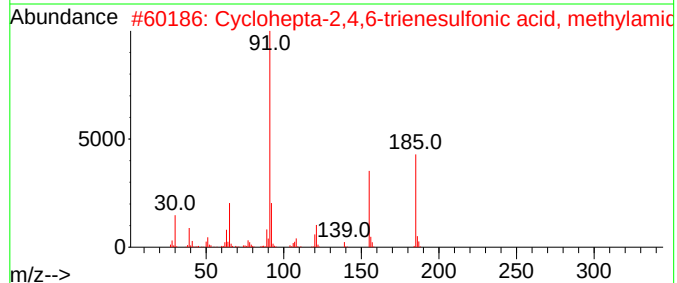
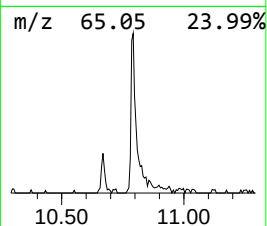
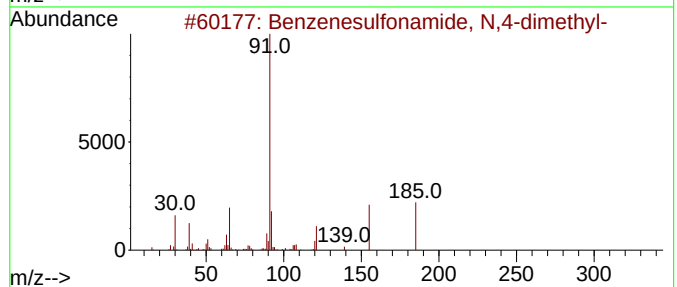
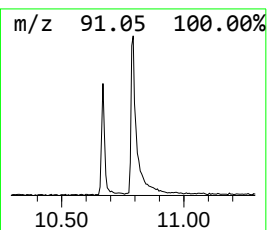
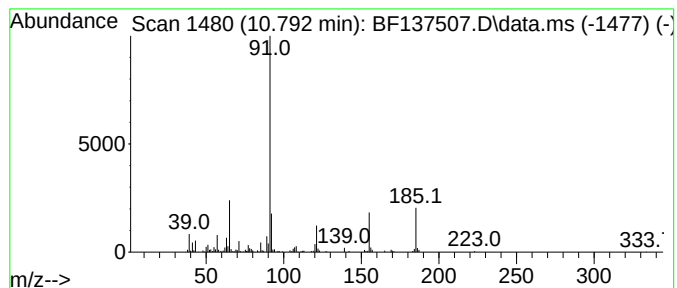
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Peak Number 3 Benzenesulfonamide, N,4-dim... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.792	3.01 ng	186345	Phenanthrene-d10	11.374

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzenesulfonamide, N,4-dimethyl-	185	C8H11NO2S	000640-61-9	96
2			Cyclohepta-2,4,6-trienesulfonic ...	185	C8H11NO2S	1000187-28-7	46
3			4-Toluenesulfonylmethyl isocyanide	195	C9H9NO2S	036635-61-7	43
4			(O-p-Tosylisonitroso)malononitrile	249	C10H7N3O3S	020893-01-0	43
5			p-Toluenesulfonylacetonitrile	195	C9H9NO2S	005697-44-9	43



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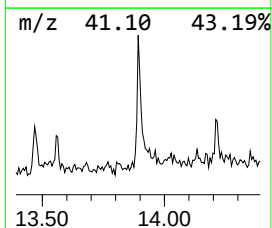
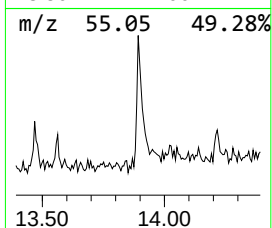
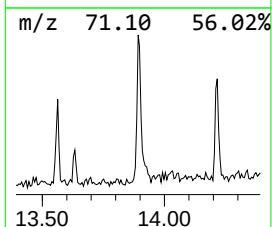
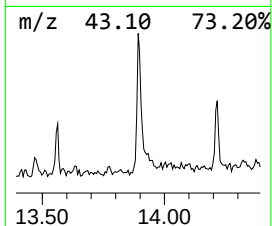
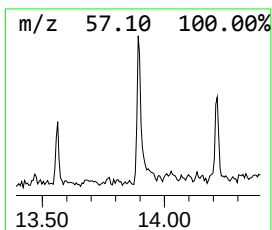
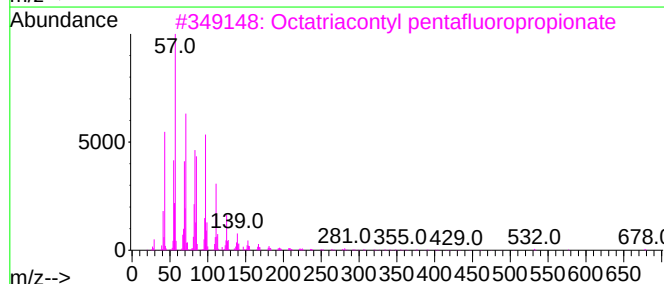
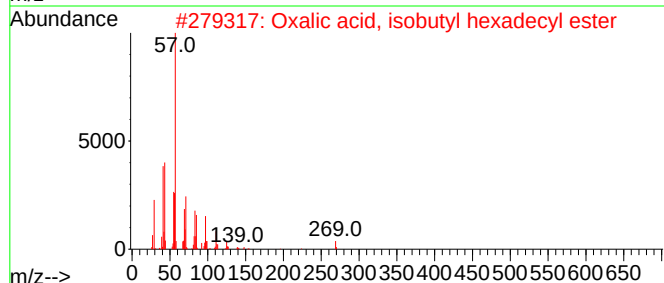
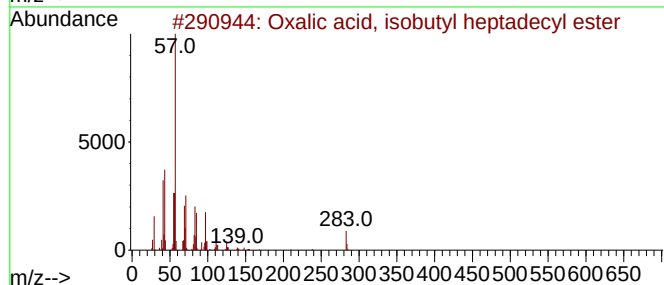
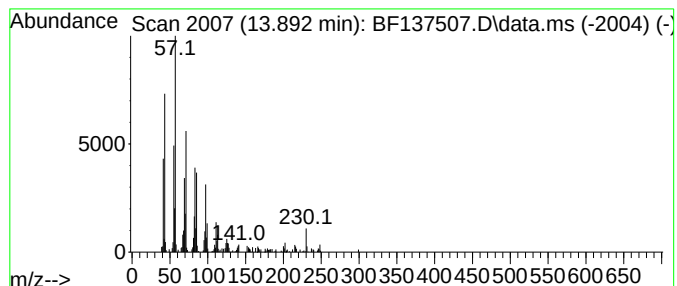
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Peak Number 4 Oxalic acid, isobutyl hepta... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.892	3.42 ng	167993	Chrysene-d12	14.033

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxalic acid, isobutyl heptadecyl...	384	C23H44O4	1000309-38-2	87
2			Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	87
3			Octatriacontyl pentafluoropropio...	697	C41H77F5O2	1000351-89-1	86
4			Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	83
5			Oxalic acid, isobutyl octadecyl ...	398	C24H46O4	1000309-38-3	80



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propylene Glycol	3.416	5.1	ng	224549	1	6.845	874291	20.0
unknown9.986	9.986	47.0	ng	3051950	3	9.875	1299940	20.0
Benzenesulfonam...	10.792	3.0	ng	186345	4	11.374	1238450	20.0
Oxalic acid, is...	13.892	3.4	ng	167993	5	14.033	983666	20.0