

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP012423\
 Data File : BP013575.D
 Acq On : 24 Jan 2023 17:36
 Operator : CG/JU
 Sample : 01190-02
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 PE-1D

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_P\Methods\8270E-BP012323.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP013575.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.222	3	6	21	rVB	1866711	2274197	15.16%	2.162%
2	5.216	338	345	355	rBV	2306183	3225235	21.51%	3.066%
3	5.687	417	425	436	rBV	5423753	8012314	53.43%	7.617%
4	7.305	689	700	711	rBV	5055057	8267500	55.13%	7.860%
5	8.157	838	845	852	rBV	1396782	2215976	14.78%	2.107%
6	9.328	1037	1044	1053	rBV	3032959	5145455	34.31%	4.892%
7	10.987	1317	1326	1334	rBV	1813314	3112592	20.76%	2.959%
8	13.422	1732	1740	1750	rBV	8013189	11647949	77.67%	11.073%
9	14.792	1967	1973	1983	rBV	2649045	3901692	26.02%	3.709%
10	16.145	2197	2203	2211	rBV	467370	641176	4.28%	0.610%
11	16.281	2219	2226	2240	rBV	5412614	7752934	51.70%	7.370%
12	17.545	2435	2441	2446	rBV	3240711	4581845	30.55%	4.356%
13	17.586	2446	2448	2455	rVB	107859	154148	1.03%	0.147%
14	17.675	2458	2463	2468	rVB2	71338	156453	1.04%	0.149%
15	17.939	2503	2508	2521	rVB	279932	459143	3.06%	0.436%
16	18.404	2582	2587	2593	rBV	251956	409290	2.73%	0.389%
17	18.480	2595	2600	2609	rVB	521450	744414	4.96%	0.708%
18	19.533	2774	2779	2790	rVB	616326	925448	6.17%	0.880%
19	19.886	2830	2839	2849	rBV	781266	1415648	9.44%	1.346%
20	20.074	2866	2871	2877	rBV	11790242	14996360	100.00%	14.256%
21	20.745	2980	2985	2993	rBV	3181887	3900559	26.01%	3.708%
22	21.298	3075	3079	3091	rBV	757201	981914	6.55%	0.933%
23	21.516	3111	3116	3124	rBV	2948769	3851300	25.68%	3.661%
24	21.621	3126	3134	3138	rVV2	3571840	7300247	48.68%	6.940%
25	21.663	3138	3141	3151	rVB	2269322	3106833	20.72%	2.954%
26	22.498	3278	3283	3290	rVB2	544980	924599	6.17%	0.879%
27	22.957	3356	3361	3372	rVB	598955	918252	6.12%	0.873%
28	23.410	3433	3438	3443	rBV	265724	513901	3.43%	0.489%
29	23.463	3443	3447	3457	rVB	219902	440086	2.93%	0.418%
30	24.210	3567	3574	3586	rVB2	1501177	3212942	21.42%	3.054%

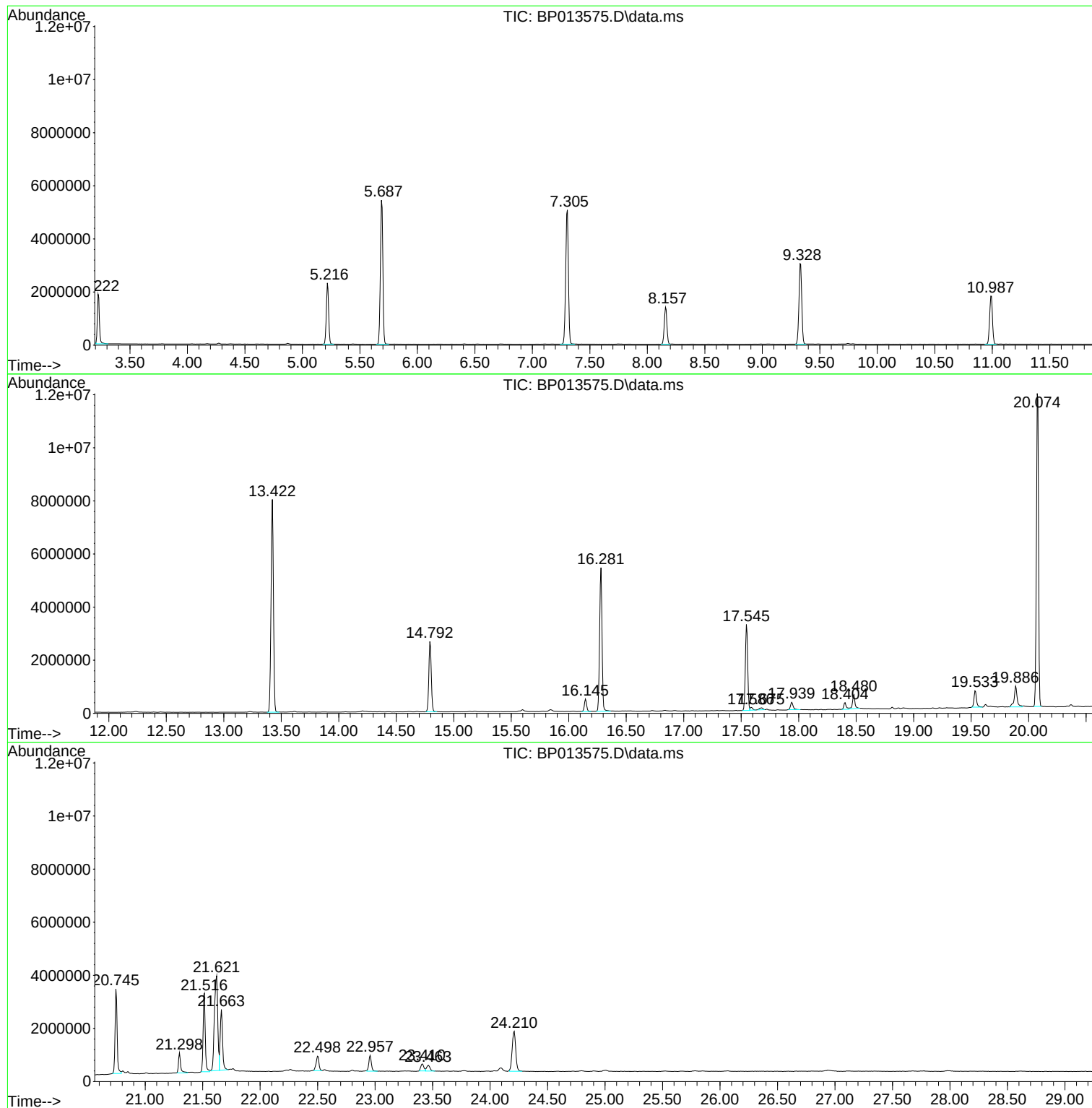
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP012323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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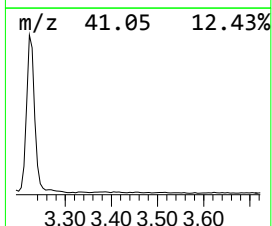
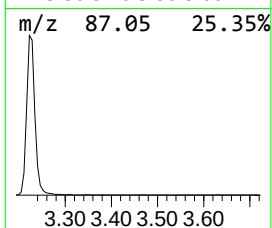
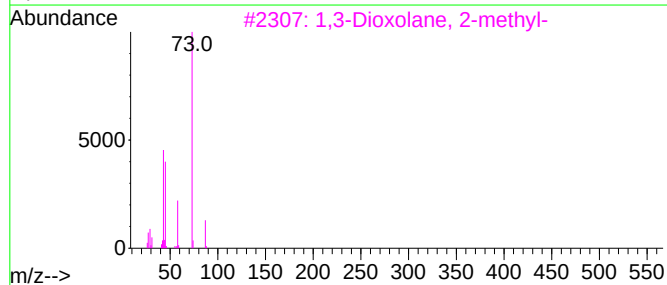
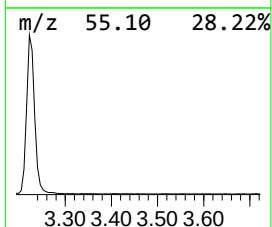
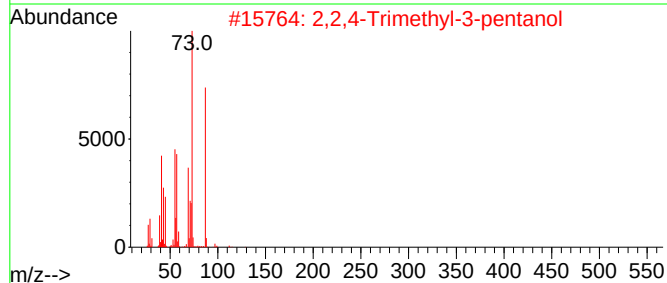
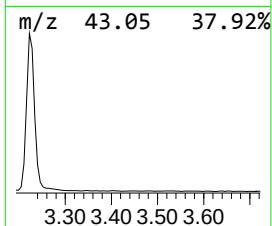
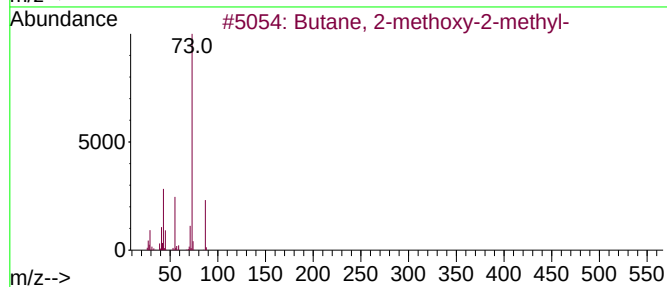
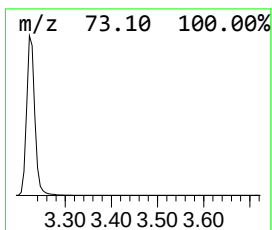
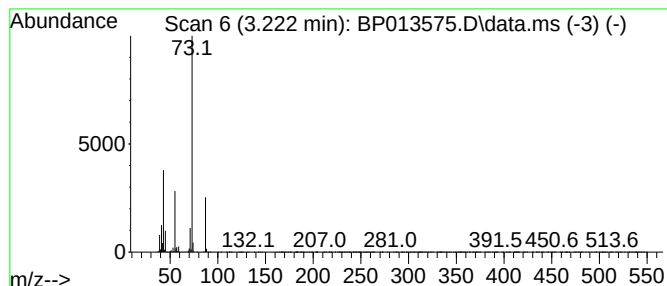
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP012323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.222	20.53 ng	2274200	1,4-Dichlorobenzene-d4	8.157

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5			Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9



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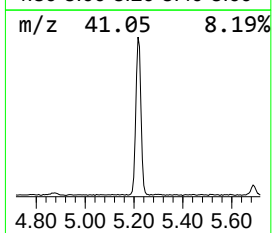
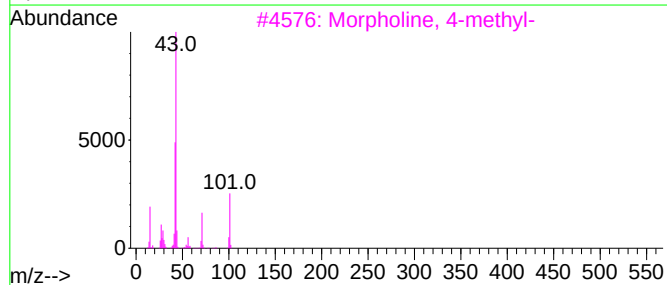
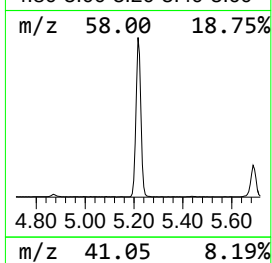
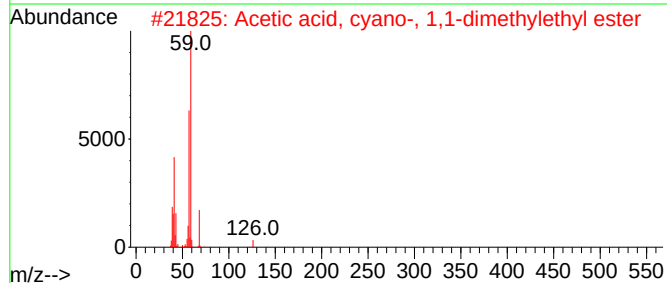
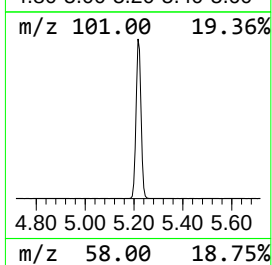
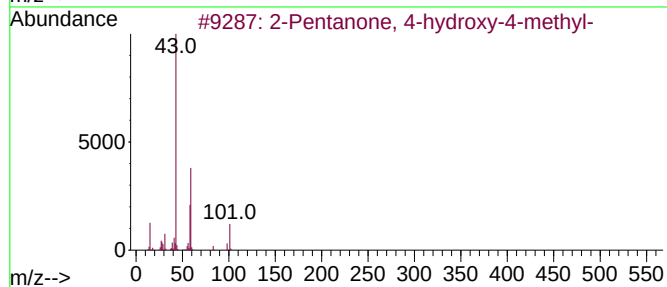
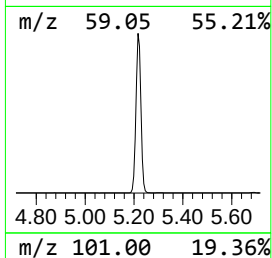
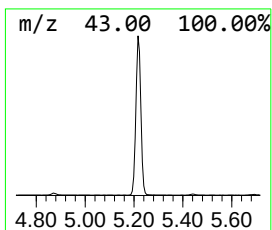
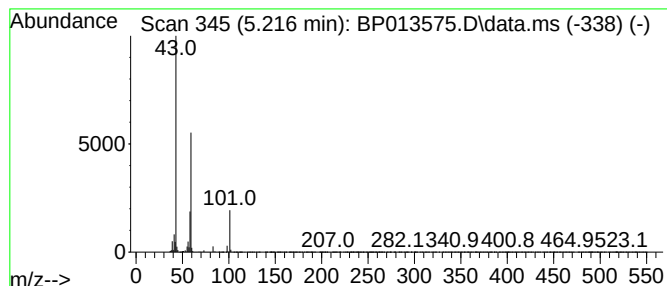
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.216	29.11 ng	3225240	1,4-Dichlorobenzene-d4	8.157

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4			Formamide, N,N-diethyl-	101	C5H11NO	000617-84-5	9
5			Acetone	58	C3H6O	000067-64-1	9



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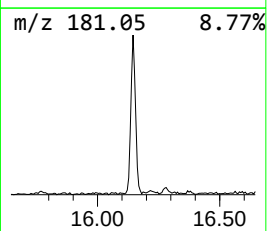
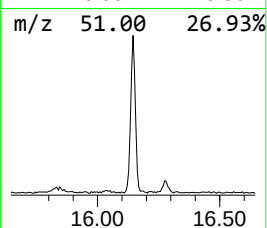
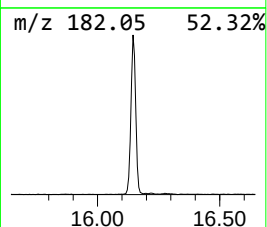
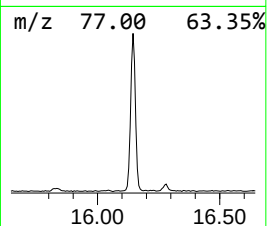
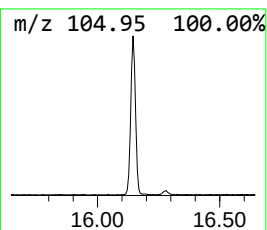
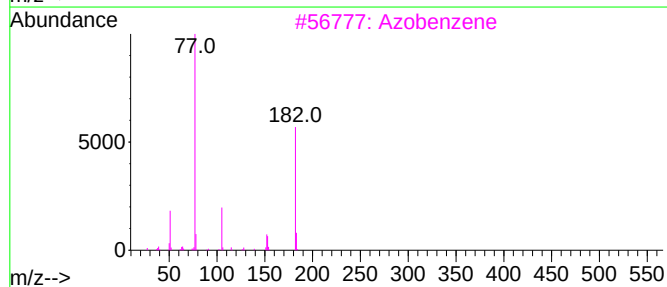
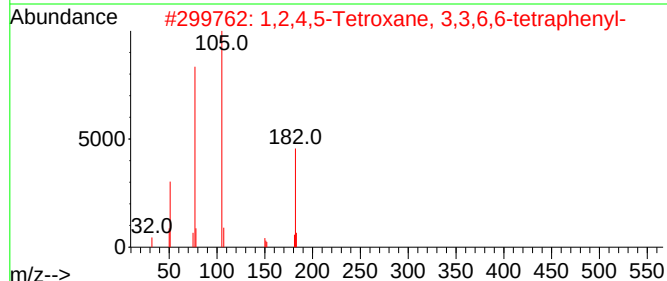
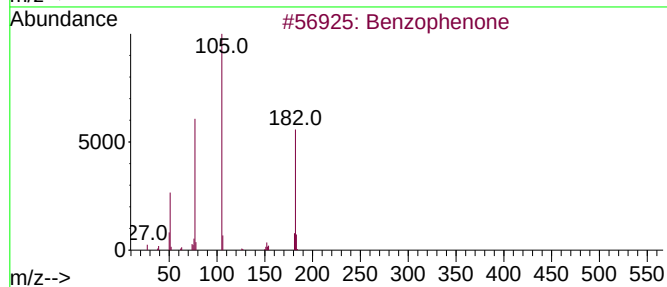
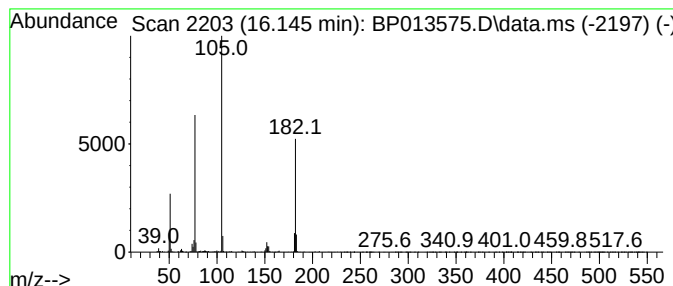
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.145	3.29 ng	641176	Acenaphthene-d10	14.792

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			1,2,4,5-Tetroxane, 3,3,6,6-tetra...	396	C26H20O4	016204-36-7	64
3			Azobenzene	182	C12H10N2	000103-33-3	59
4			Benzenamine, N-(3-pyridinylmethy...	182	C12H10N2	029722-97-2	59
5			Methanone, phenyl-2-pyridinyl-	183	C12H9NO	000091-02-1	50



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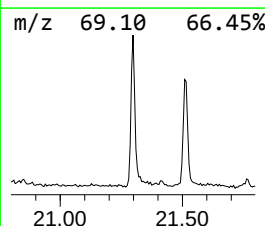
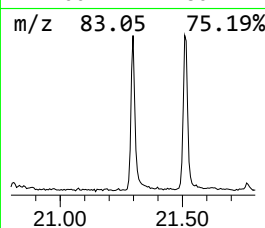
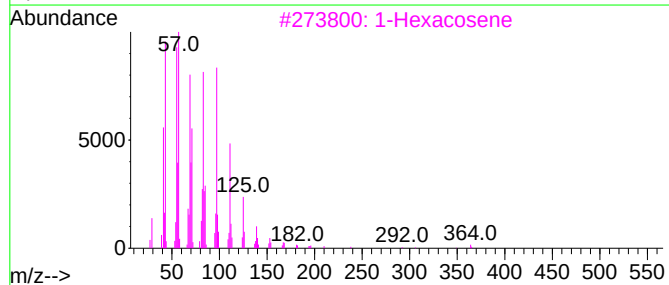
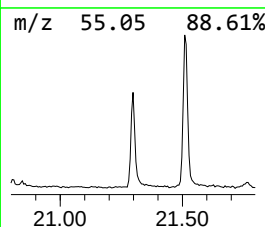
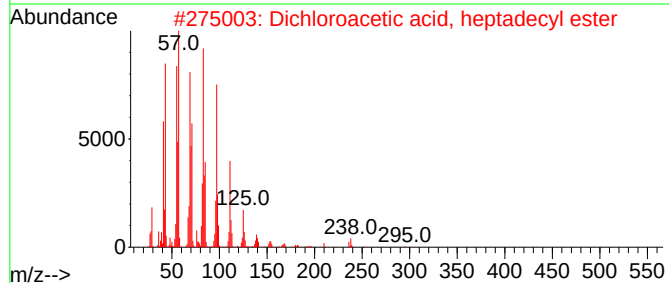
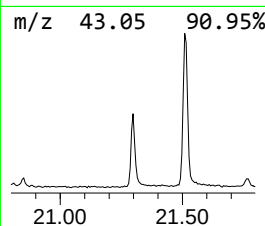
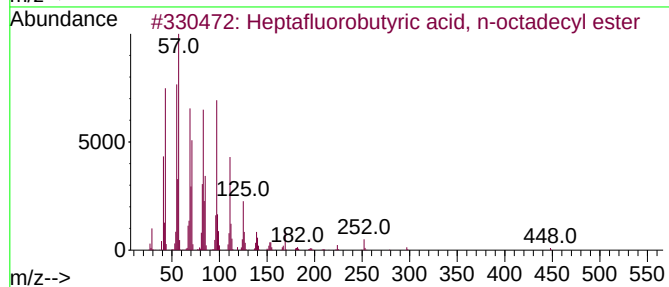
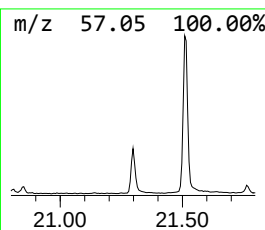
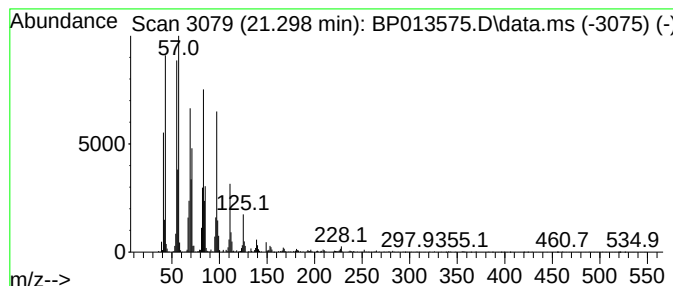
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Peak Number 4 Heptafluorobutyric acid, n-... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.298	2.69 ng	981914	Chrysene-d12	21.621

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	94
2			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
3			1-Hexacosene	364	C26H52	018835-33-1	94
4			1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
5			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94



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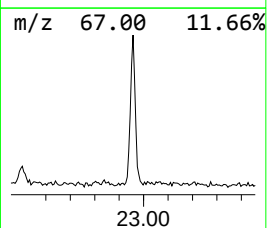
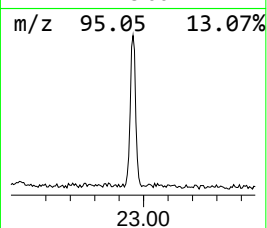
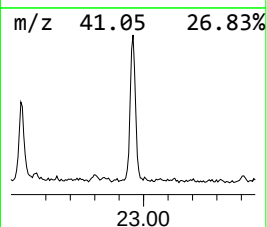
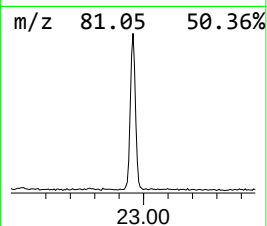
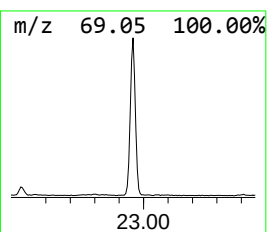
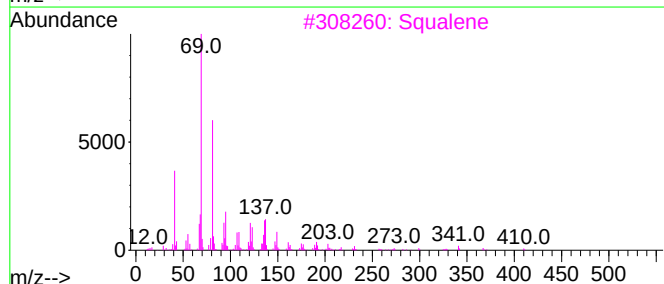
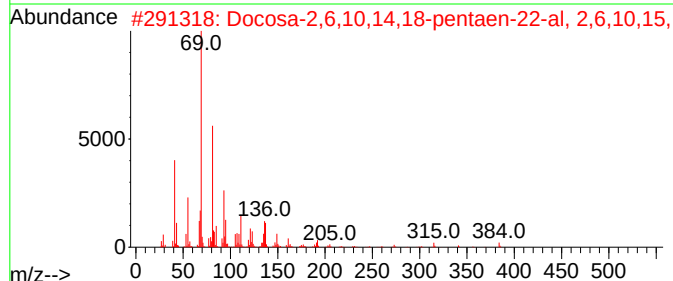
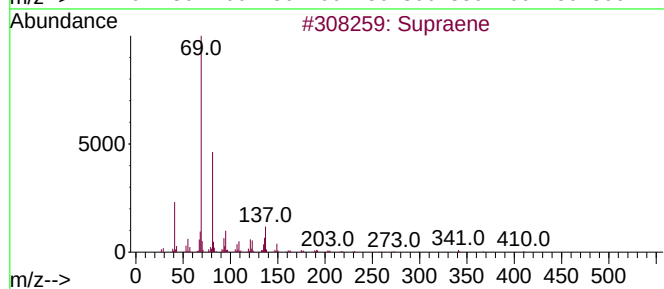
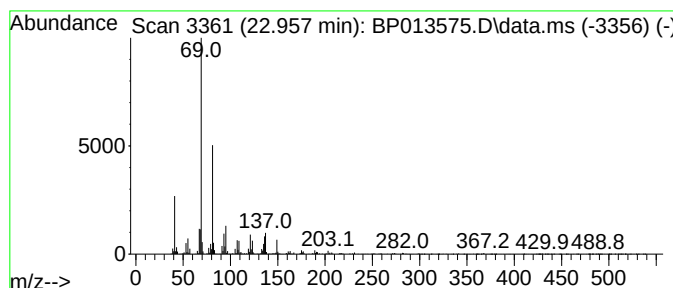
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Supraene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.957	5.72 ng	918252	Perylene-d12	24.209

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	91
2			Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	91
3			Squalene	410	C30H50	000111-02-4	90
4			(2E,6E,10E)-3,7,11,15-Tetramethy...	318	C21H34O2	125456-63-5	78
5			Farnesol (E), methyl ether	236	C16H28O	1000352-67-3	72



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	3.222	20.5	ng	2274200	1	8.157	2215980	20.0
2-Pentanone, 4-...	5.216	29.1	ng	3225240	1	8.157	2215980	20.0
Benzophenone	16.145	3.3	ng	641176	3	14.792	3901690	20.0
Heptafluorobuty...	21.298	2.7	ng	981914	5	21.621	7300250	20.0
Supraene	22.957	5.7	ng	918252	6	24.209	3212940	20.0