

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP012423\
 Data File : BP013569.D
 Acq On : 24 Jan 2023 14:00
 Operator : CG/JU
 Sample : 01214-19
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 TJRC-011823-GW-DUP

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: BP013569.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.223	3	6	25	rVB	5372282	6313815	53.96%	10.782%
2	5.217	338	345	352	rBV	642372	898578	7.68%	1.534%
3	5.687	418	425	435	rVB	1973843	2840261	24.27%	4.850%
4	7.293	692	698	708	rBV	1060374	1668967	14.26%	2.850%
5	8.158	838	845	852	rBV	912566	1460583	12.48%	2.494%
6	9.328	1037	1044	1053	rBV	2667462	4473260	38.23%	7.639%
7	10.987	1317	1326	1334	rBV	1099734	1897463	16.22%	3.240%
8	13.422	1733	1740	1751	rBV	6823166	9718807	83.06%	16.597%
9	14.069	1846	1850	1861	rBV	65074	119343	1.02%	0.204%
10	14.793	1966	1973	1988	rVB	1405473	2129249	18.20%	3.636%
11	16.145	2197	2203	2209	rBV	516988	709017	6.06%	1.211%
12	16.281	2218	2226	2236	rBV	3975443	5817388	49.72%	9.934%
13	17.545	2435	2441	2448	rBV	1645801	2299103	19.65%	3.926%
14	18.398	2582	2586	2592	rBV	135382	208141	1.78%	0.355%
15	19.628	2791	2795	2803	rBV2	97285	153107	1.31%	0.261%
16	20.075	2866	2871	2877	rBV	9621680	11700753	100.00%	19.981%
17	21.298	3075	3079	3088	rBV	193558	321694	2.75%	0.549%
18	21.622	3129	3134	3140	rBV	1926712	2540857	21.72%	4.339%
19	22.957	3357	3361	3367	rVB	212656	313406	2.68%	0.535%
20	24.210	3567	3574	3585	rVB2	1381773	2975069	25.43%	5.080%

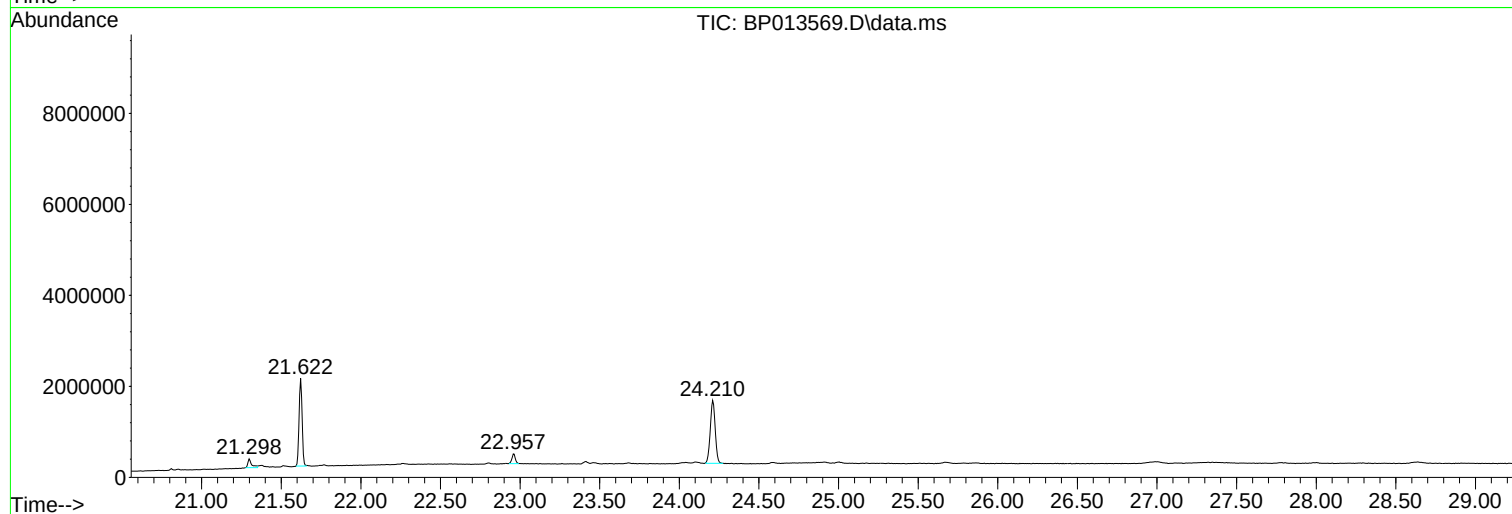
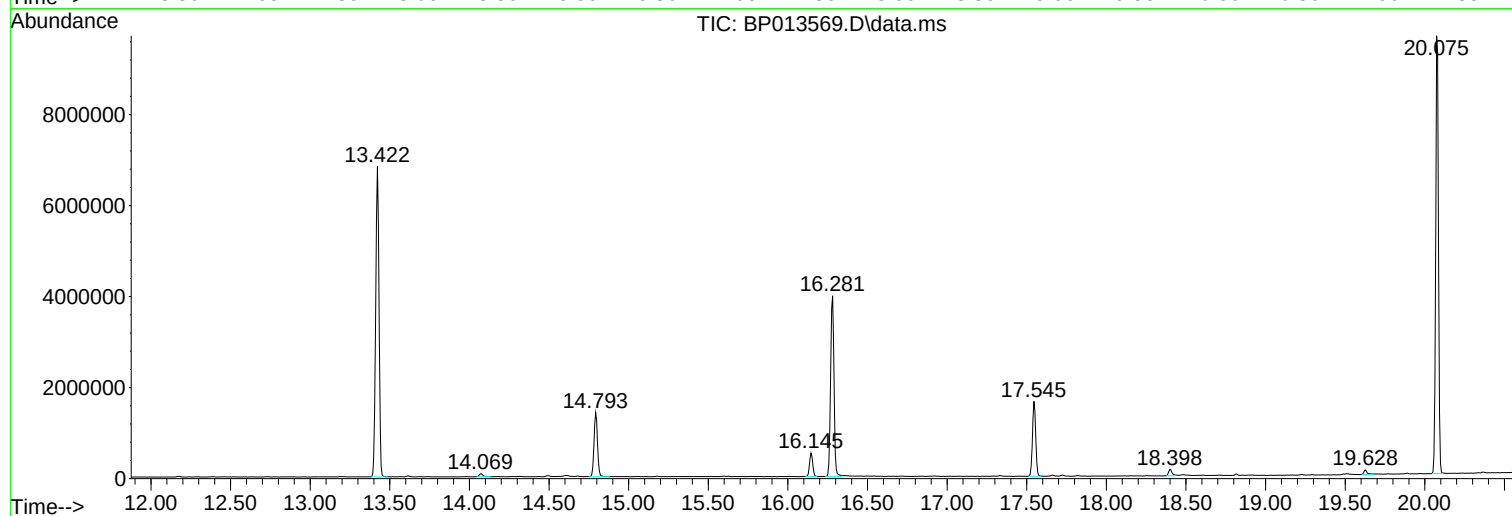
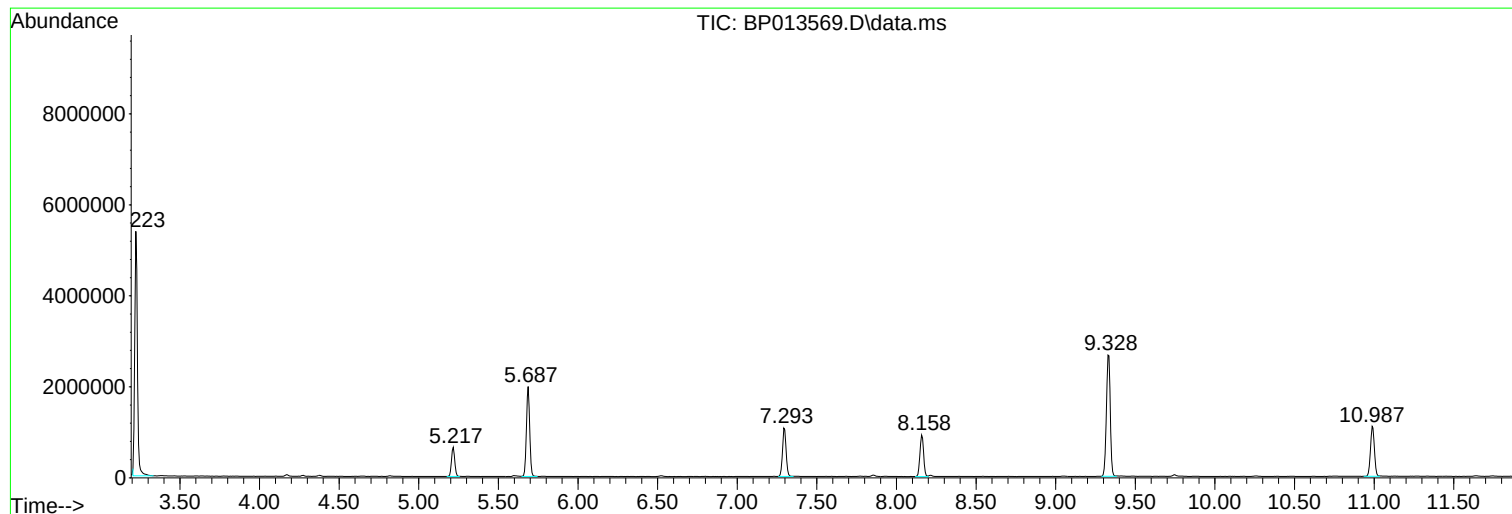
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP012323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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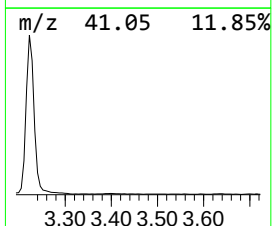
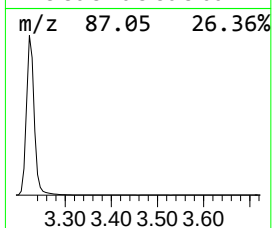
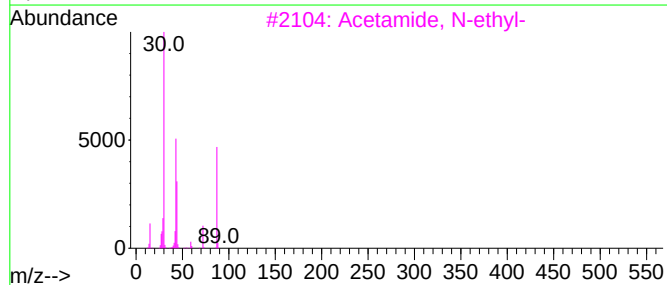
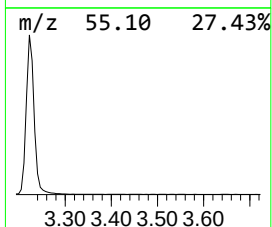
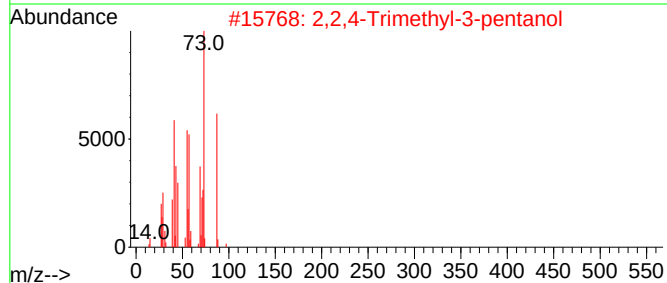
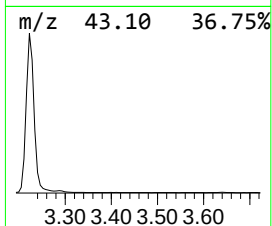
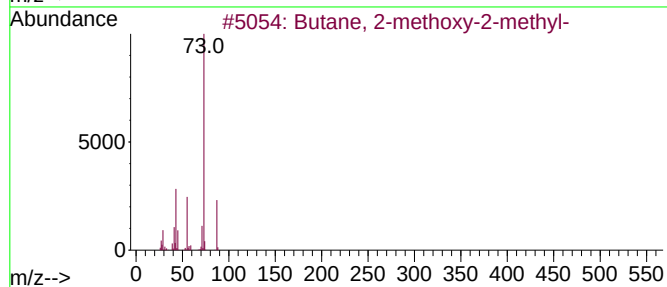
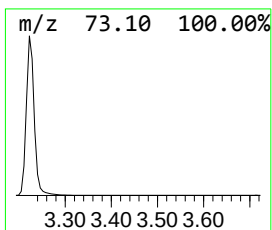
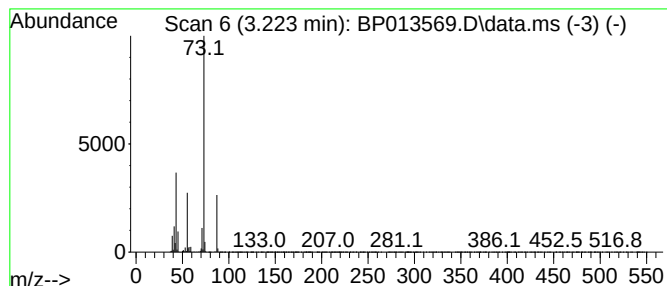
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.223	86.46 ng	6313820	1,4-Dichlorobenzene-d4	8.158

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			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9



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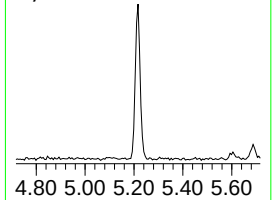
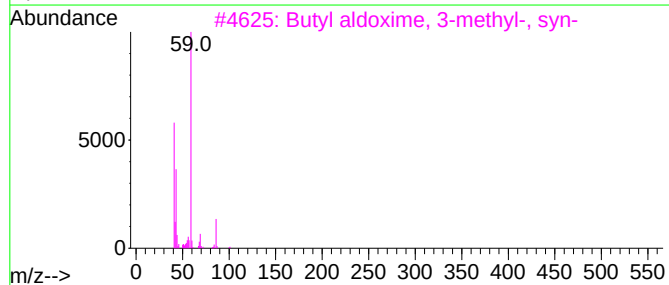
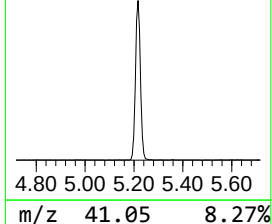
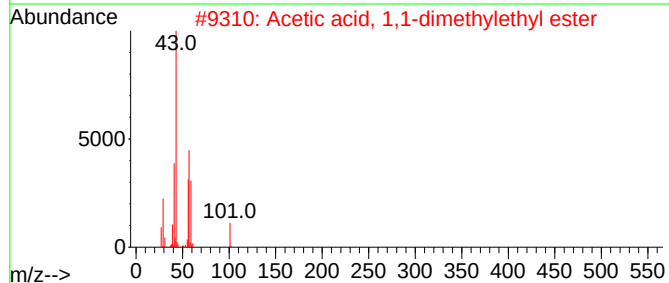
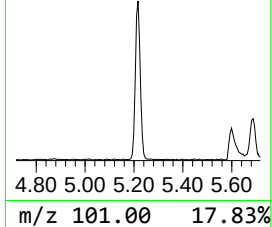
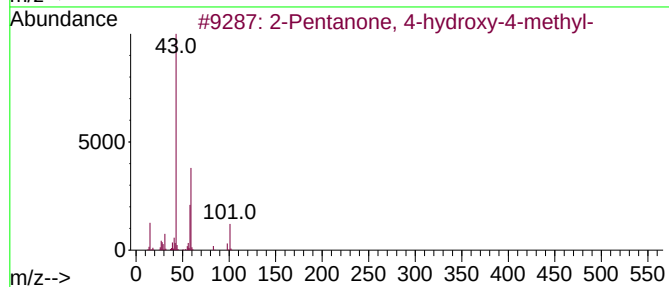
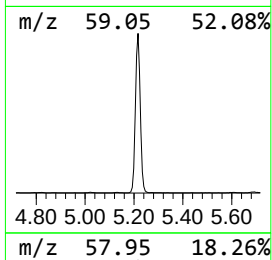
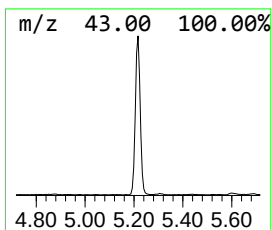
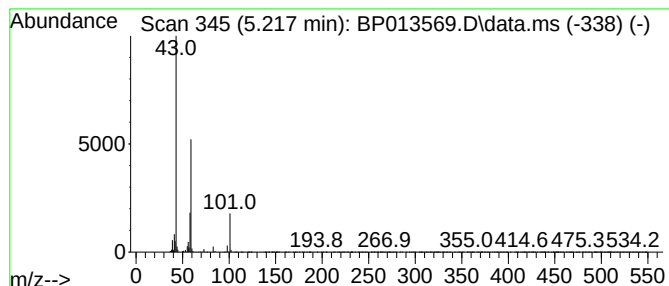
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP012323.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.217	12.30 ng	898578	1,4-Dichlorobenzene-d4	8.158

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
3			Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	23
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12



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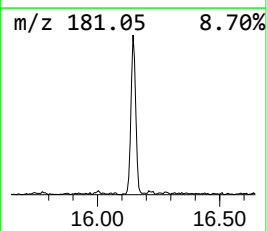
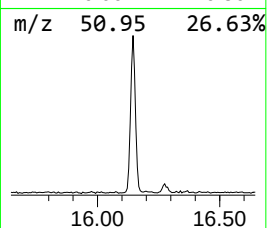
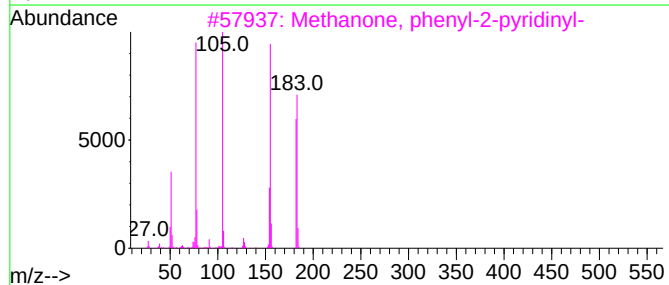
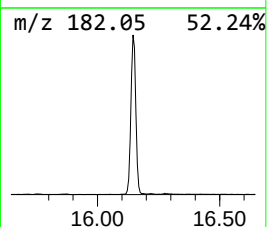
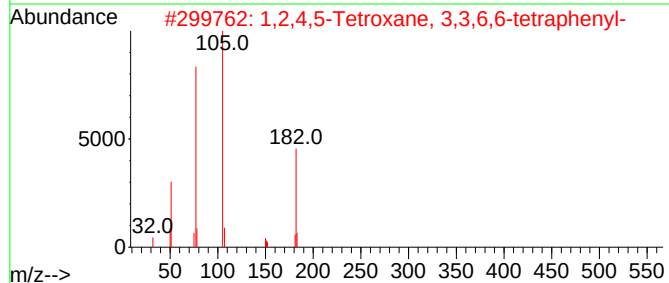
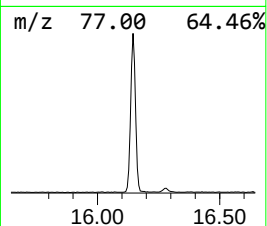
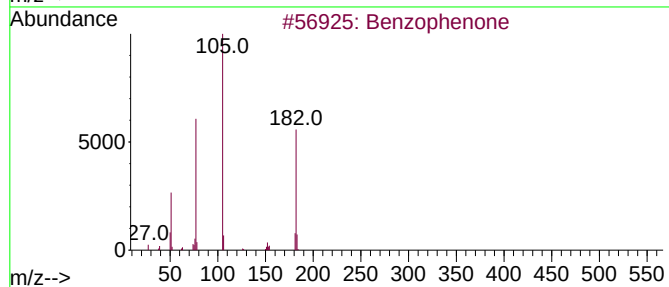
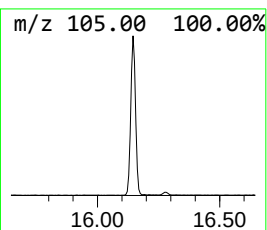
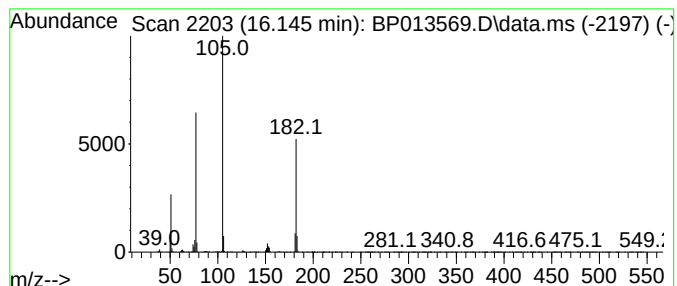
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.145	6.66 ng	709017	Acenaphthene-d10	14.793

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			Methanone, phenyl-2-pyridinyl-	183	C12H9NO	000091-02-1	56
4			Benzenamine, N-(3-pyridinylmethy...	182	C12H10N2	029722-97-2	53
5			Azobenzene	182	C12H10N2	000103-33-3	42



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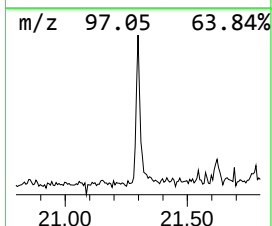
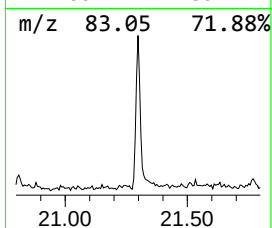
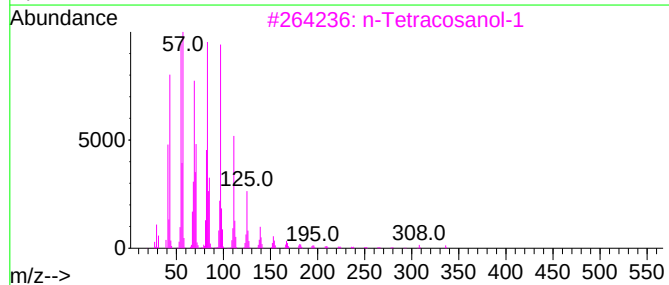
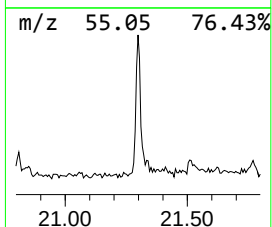
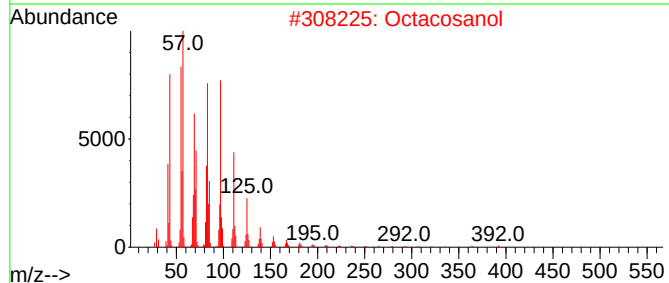
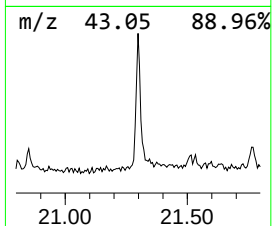
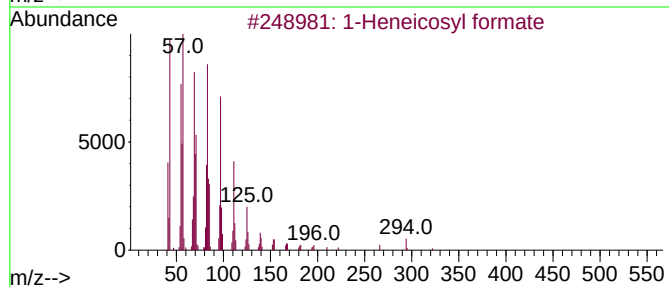
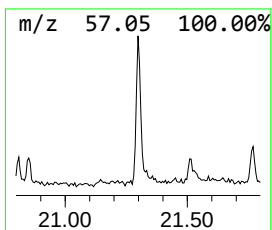
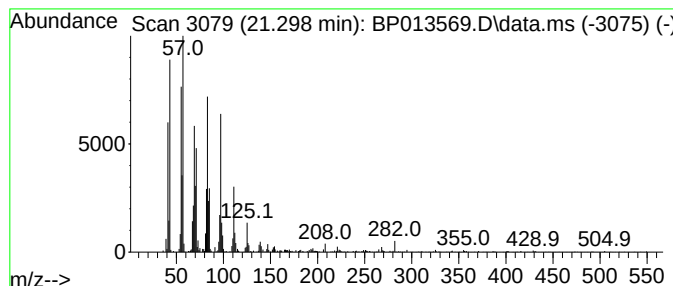
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Peak Number 4 1-Heneicosyl formate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.298	2.53 ng	321694	Chrysene-d12	21.622

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosyl formate	340	C22H44O2	077899-03-7	93
2			Octacosanol	410	C28H58O	000557-61-9	91
3			n-Tetracosanol-1	354	C24H50O	000506-51-4	90
4			Cyclotetracosane	336	C24H48	000297-03-0	90
5			Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	90



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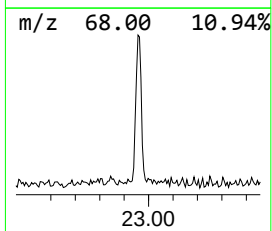
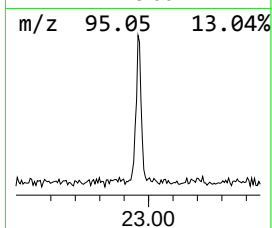
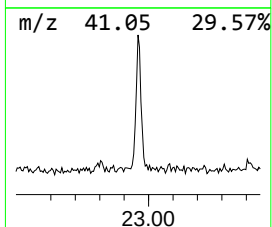
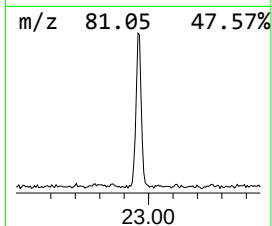
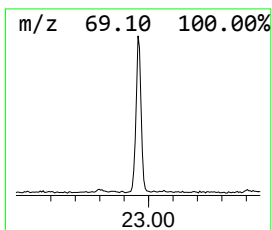
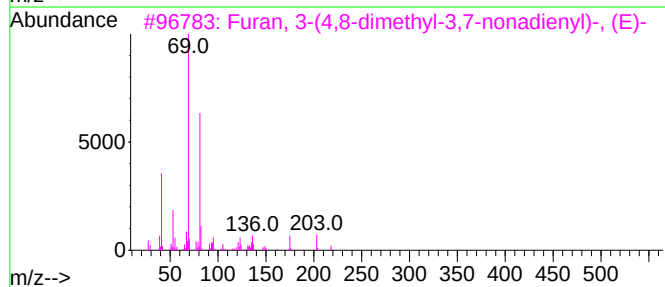
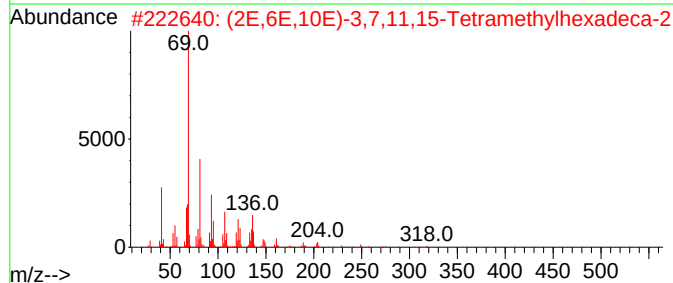
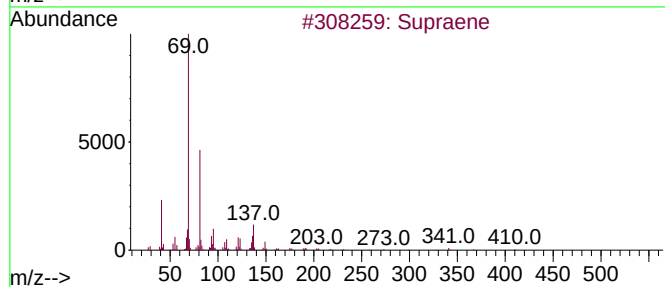
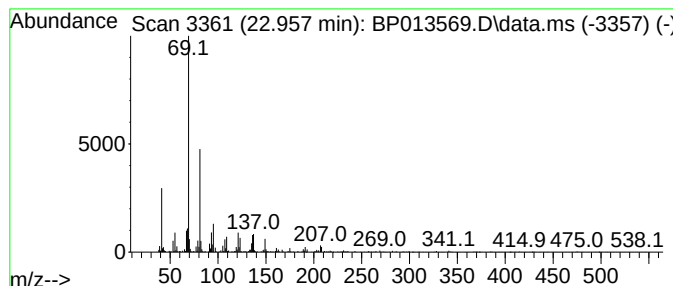
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Supraene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.957	2.11 ng	313406	Perylene-d12	24.210

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	91
2			(2E,6E,10E)-3,7,11,15-Tetramethy...	318	C21H34O2	125456-63-5	78
3			Furan, 3-(4,8-dimethyl-3,7-nonad...	218	C15H22O	023262-34-2	72
4			trans-Farnesol	222	C15H26O	000106-28-5	72
5			1,3-Dioxolan-2-one, 3-methyl-3-(...	264	C16H24O3	336879-76-6	64



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	3.223	86.5	ng	6313820	1	8.158	1460580	20.0
2-Pentanone, 4-...	5.217	12.3	ng	898578	1	8.158	1460580	20.0
Benzophenone	16.145	6.7	ng	709017	3	14.793	2129250	20.0
1-Heneicosyl fo...	21.298	2.5	ng	321694	5	21.622	2540860	20.0
Supraene	22.957	2.1	ng	313406	6	24.210	2975070	20.0