

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112222\
 Data File : BF131346.D
 Acq On : 22 Nov 2022 23:53
 Operator : CG\JU
 Sample : N5740-01
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MH-12

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-BF112122.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131346.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.293	26	35	44	rVB	1052836	1415106	50.72%	7.086%
2	2.399	48	53	60	rBV	56086	70910	2.54%	0.355%
3	5.193	523	528	536	rVB	443792	572523	20.52%	2.867%
4	5.575	588	593	596	rBV	2528011	2636524	94.49%	13.202%
5	6.581	757	764	767	rBV	2384959	2624910	94.08%	13.144%
6	6.963	825	829	832	rBV	835573	631777	22.64%	3.164%
7	7.528	920	925	928	rBV	1713602	1713571	61.41%	8.581%
8	8.251	1044	1048	1051	rBV	986229	796972	28.56%	3.991%
9	9.333	1227	1232	1235	rBV	3380450	2790206	100.00%	13.972%
10	10.016	1344	1348	1351	rBV	1109069	857569	30.73%	4.294%
11	10.733	1466	1470	1473	rBV	73800	59429	2.13%	0.298%
12	10.810	1478	1483	1486	rBV	1808626	1588940	56.95%	7.957%
13	11.510	1599	1602	1606	rBV	852543	731681	26.22%	3.664%
14	12.033	1687	1691	1697	rBV	90196	97327	3.49%	0.487%
15	13.110	1869	1874	1877	rBV	2008556	1848259	66.24%	9.255%
16	14.139	2034	2049	2050	rBV9	28916	109447	3.92%	0.548%
17	14.168	2050	2054	2069	rVB	630555	608209	21.80%	3.046%
18	14.327	2079	2081	2091	rVB	26835	35417	1.27%	0.177%
19	14.639	2129	2134	2140	rVB	27142	34238	1.23%	0.171%
20	15.051	2200	2204	2210	rVB	147361	153943	5.52%	0.771%
21	15.710	2310	2316	2321	rBV	460970	593271	21.26%	2.971%

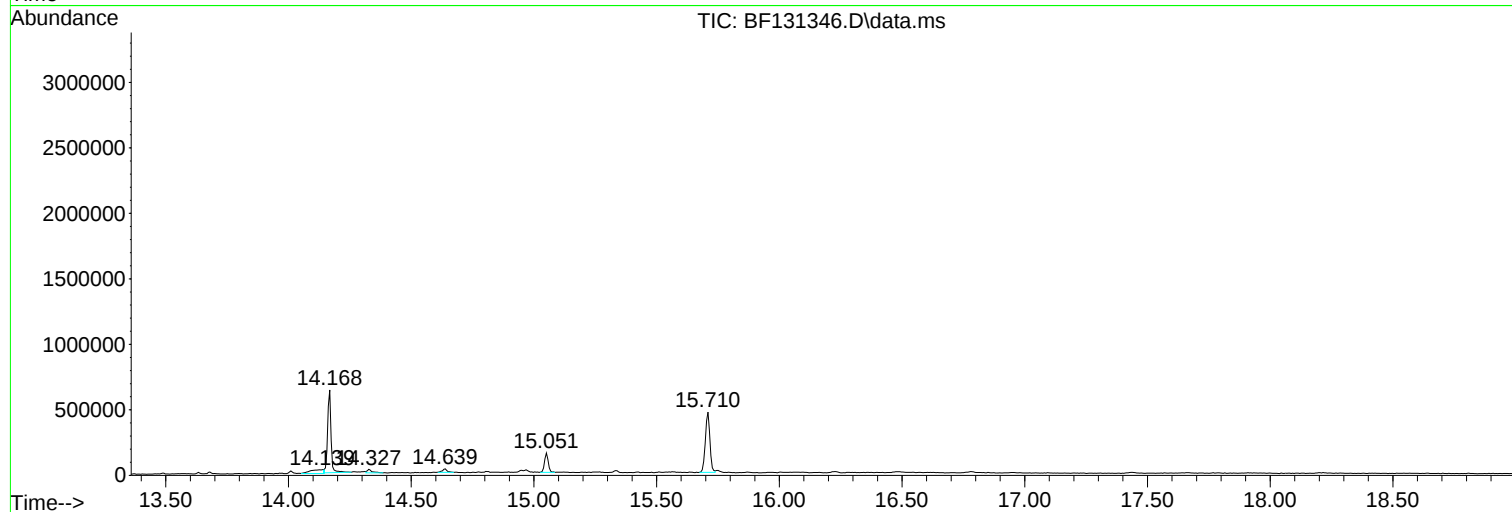
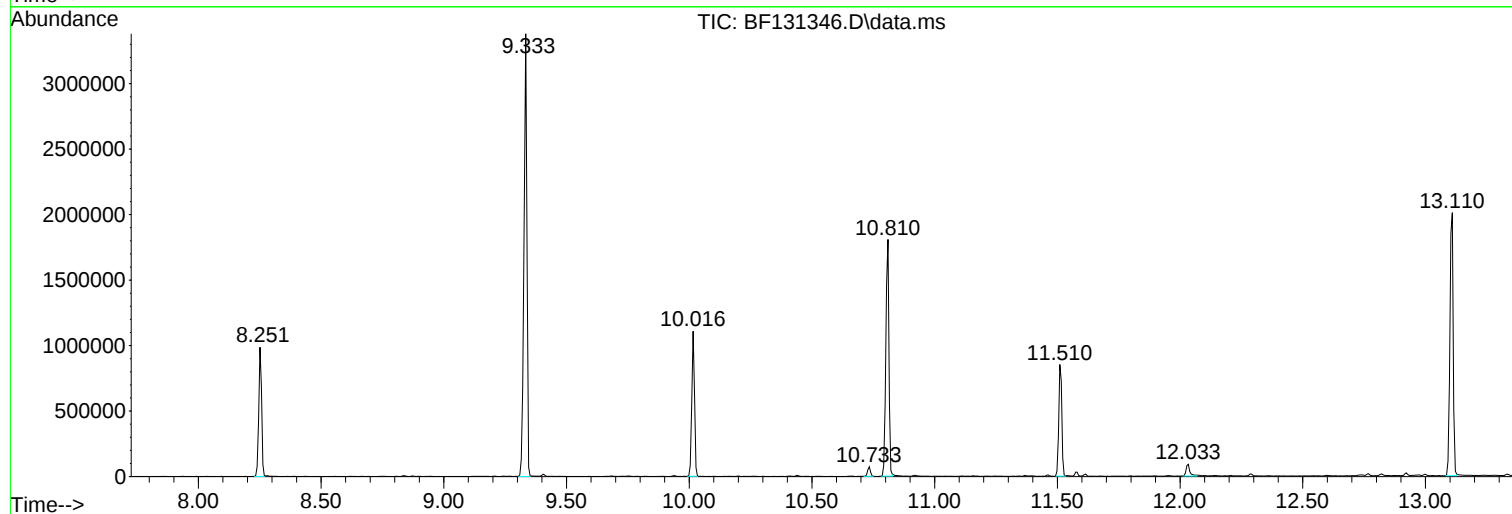
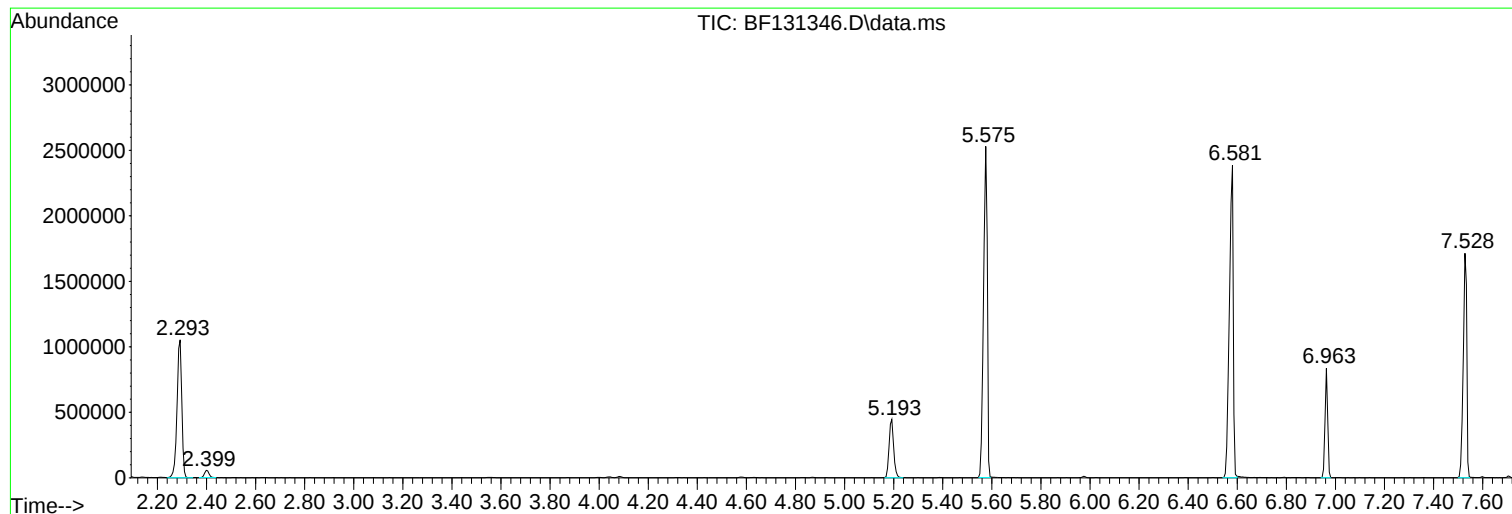
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Data File : BF131346.D
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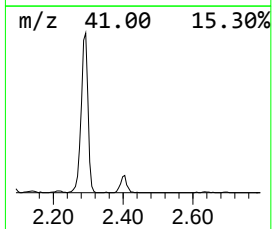
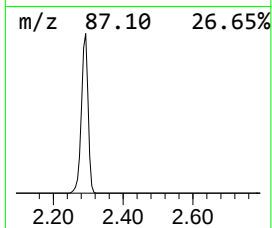
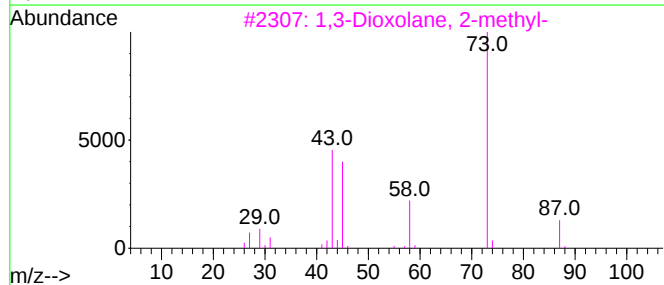
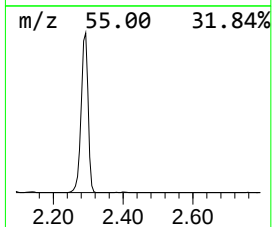
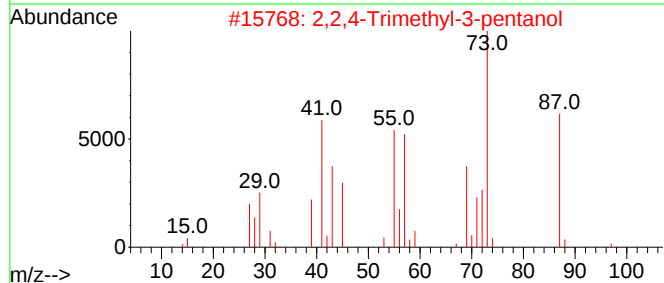
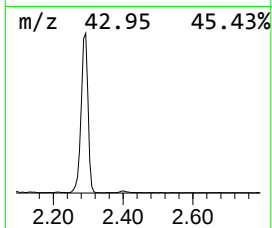
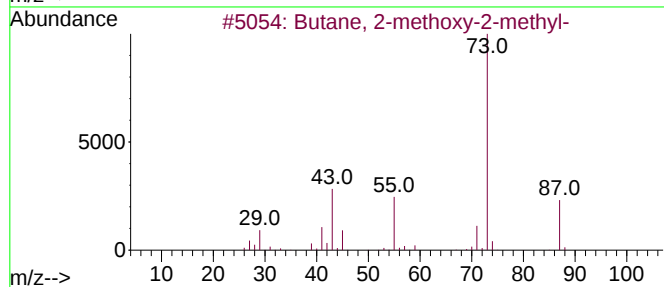
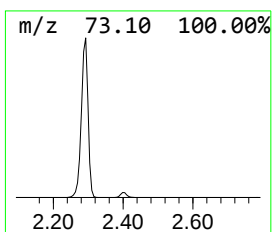
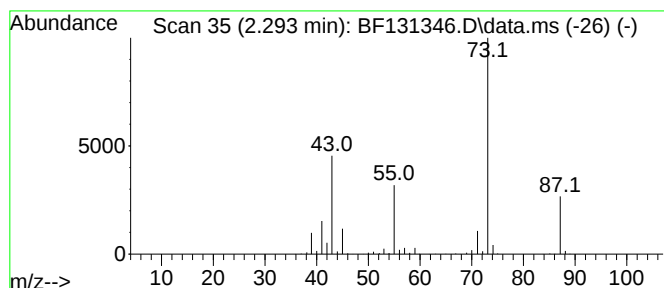
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.293	44.80 ng	1415110	1,4-Dichlorobenzene-d4	6.963

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	40
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17



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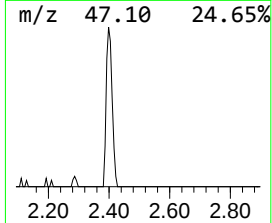
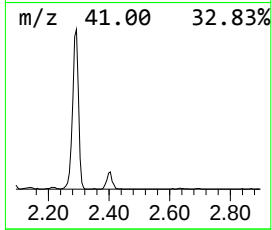
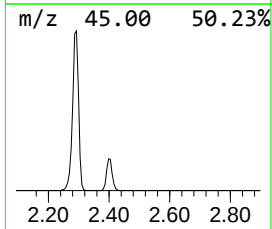
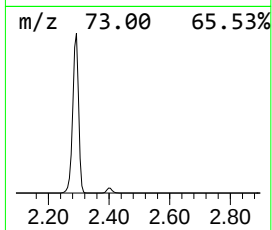
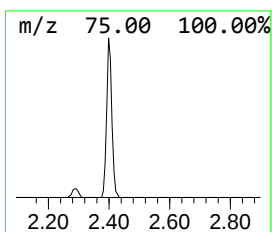
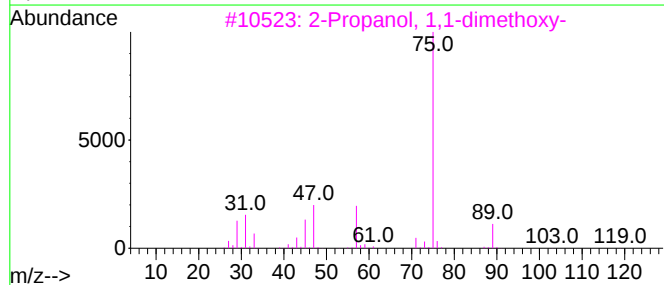
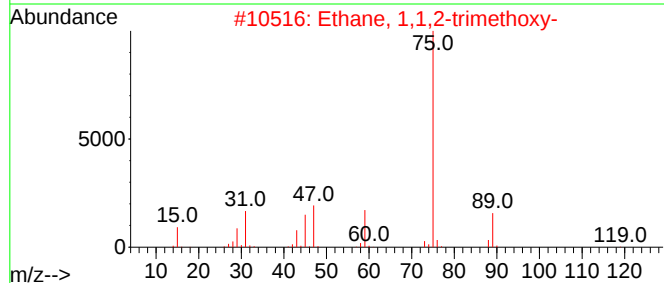
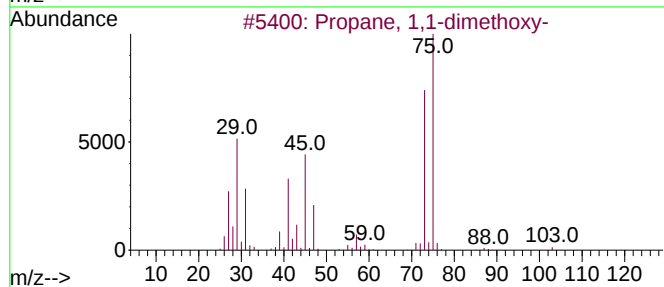
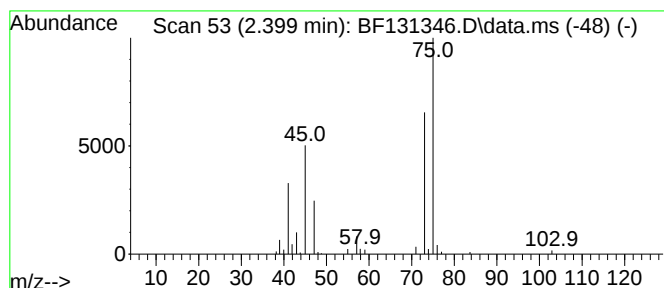
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.399	2.24 ng	70910	1,4-Dichlorobenzene-d4	6.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	64
2			Ethane, 1,1,2-trimethoxy-	120	C5H12O3	024332-20-5	42
3			2-Propanol, 1,1-dimethoxy-	120	C5H12O3	042919-42-6	42
4			Methane, trimethoxy-	106	C4H10O3	000149-73-5	40
5			Ethane, 2-chloro-1,1-dimethoxy-	124	C4H9ClO2	000097-97-2	9



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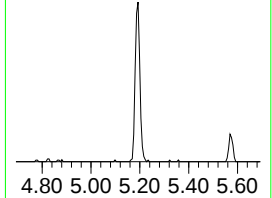
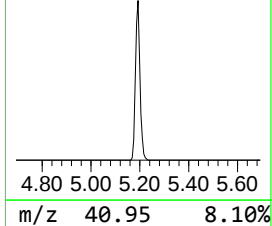
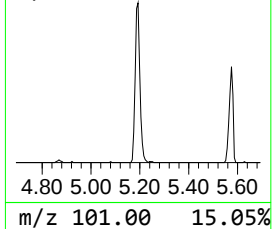
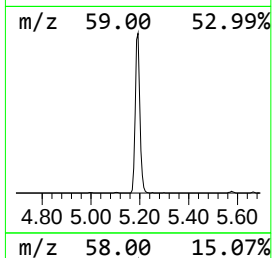
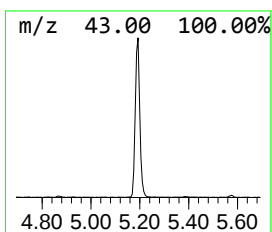
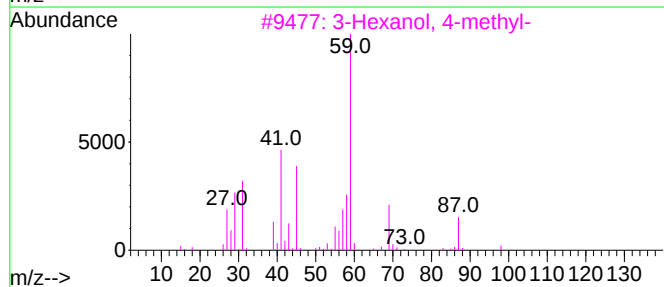
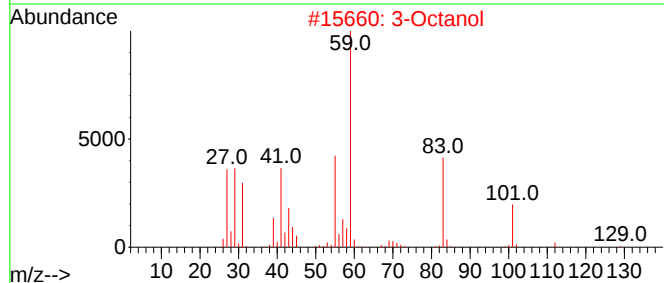
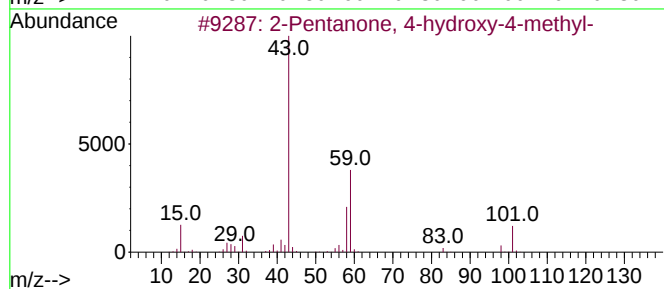
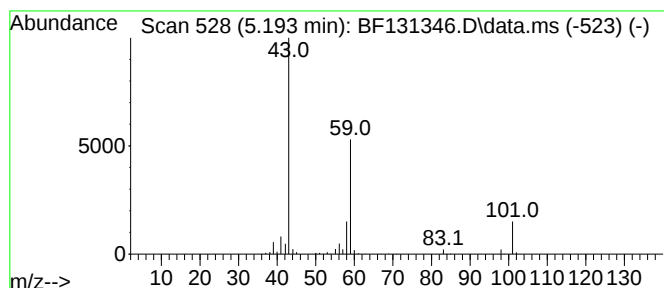
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.193	18.12 ng	572523	1,4-Dichlorobenzene-d4	6.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			3-Octanol	130	C8H18O	000589-98-0	33
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27



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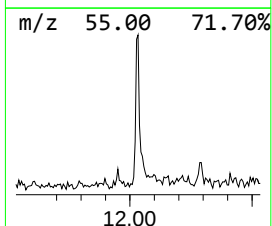
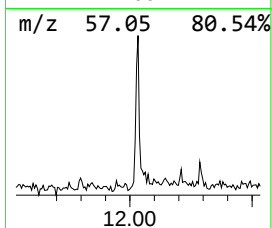
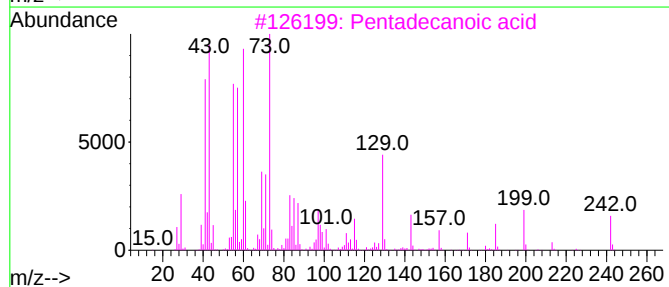
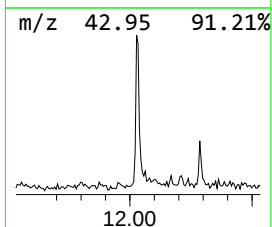
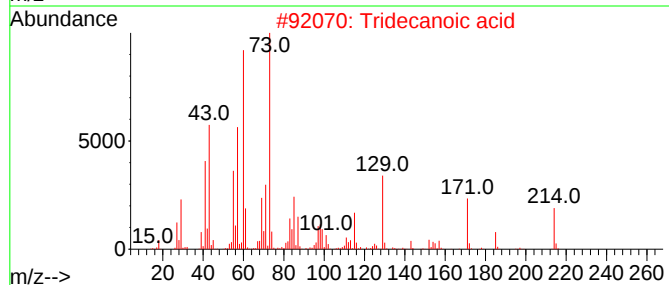
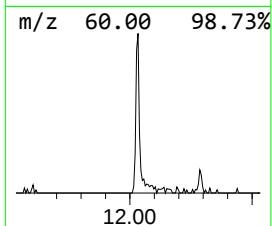
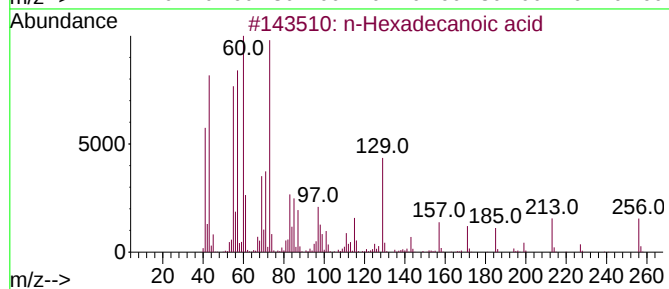
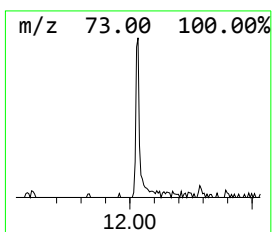
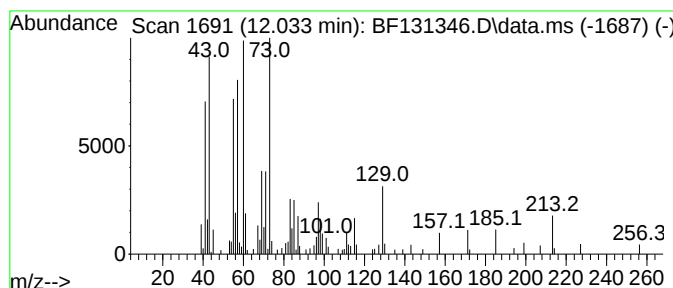
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.033	2.66 ng	97327	Phenanthrene-d10	11.510

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
2			Tridecanoic acid	214	C13H26O2	000638-53-9	90
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5			n-Decanoic acid	172	C10H20O2	000334-48-5	58



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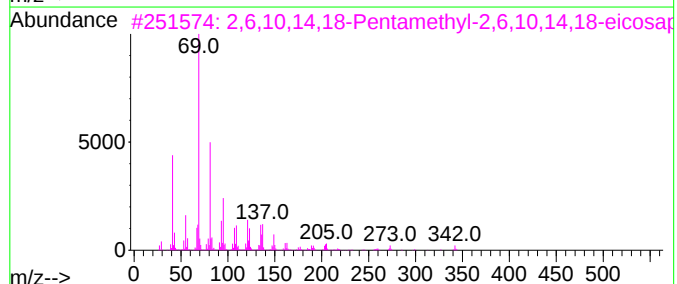
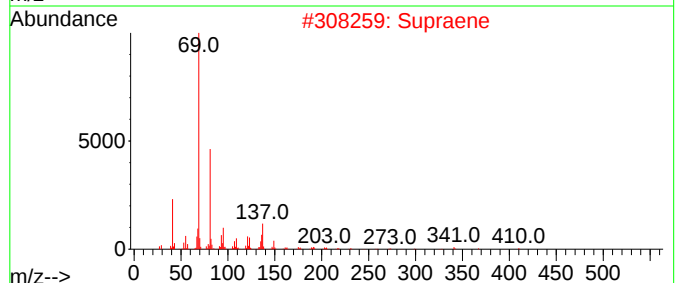
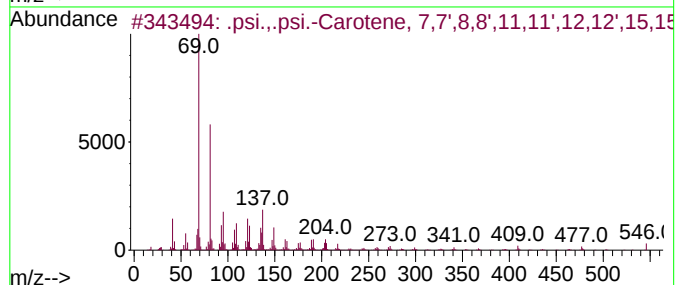
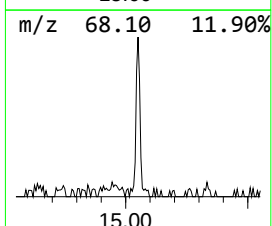
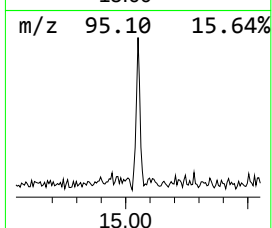
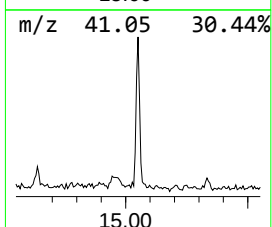
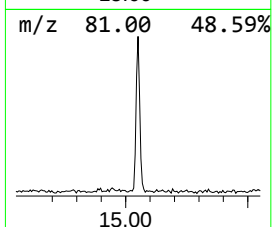
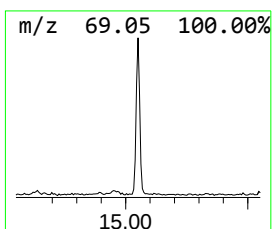
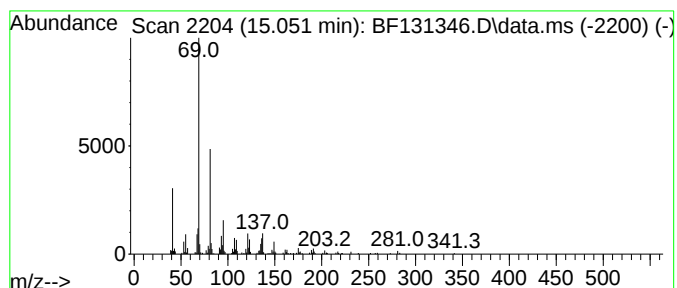
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 .psi.,.psi.-Carotene, 7,7',... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.051	5.19 ng	153943	Perylene-d12	15.710	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	83
2	Supraene	410	C30H50	007683-64-9	80
3	2,6,10,14,18-Pentamethyl-2,6,10,...	342	C25H42	075581-03-2	78
4	2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	72
5	Farnesol isomer a	222	C15H26O	1000108-92-4	72



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.293	44.8	ng	1415110	1	6.963	631777	20.0
Propane, 1,1-di...	2.399	2.2	ng	70910	1	6.963	631777	20.0
2-Pentanone, 4-...	5.193	18.1	ng	572523	1	6.963	631777	20.0
n-Hexadecanoic ...	12.033	2.7	ng	97327	4	11.510	731681	20.0
.psi.,.psi.-Car...	15.051	5.2	ng	153943	6	15.710	593271	20.0