

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121622\
 Data File : BF131680.D
 Acq On : 16 Dec 2022 22:34
 Operator : CG\JU
 Sample : N6037-24
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RB-28-(5-7)

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-BF120822.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131680.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.128	3	7	14	rVB	365502	442754	19.47%	2.917%
2	5.087	506	510	522	rVB	230628	283152	12.45%	1.865%
3	5.492	574	579	582	rBV	2012517	1871900	82.33%	12.331%
4	6.510	747	752	755	rBV	1971070	1892943	83.26%	12.469%
5	6.881	811	815	818	rBV	595379	477633	21.01%	3.146%
6	7.445	906	911	914	rBV	1260864	1206043	53.04%	7.945%
7	8.169	1030	1034	1037	rBV	753760	590801	25.98%	3.892%
8	9.251	1213	1218	1221	rBV	2563651	2194776	96.53%	14.458%
9	9.933	1330	1334	1337	rBV	799490	683861	30.08%	4.505%
10	10.651	1452	1456	1459	rBV	121436	96913	4.26%	0.638%
11	10.727	1464	1469	1472	rBV	1516520	1408063	61.93%	9.275%
12	11.427	1584	1588	1591	rBV	847967	718206	31.59%	4.731%
13	13.021	1854	1859	1862	rBV	2690464	2273651	100.00%	14.977%
14	13.921	2008	2012	2014	rBV2	29728	40042	1.76%	0.264%
15	14.080	2035	2039	2042	rVB	523501	493152	21.69%	3.249%
16	14.939	2181	2185	2190	rVB	52670	52933	2.33%	0.349%
17	15.580	2289	2294	2304	rVB	351743	453995	19.97%	2.991%

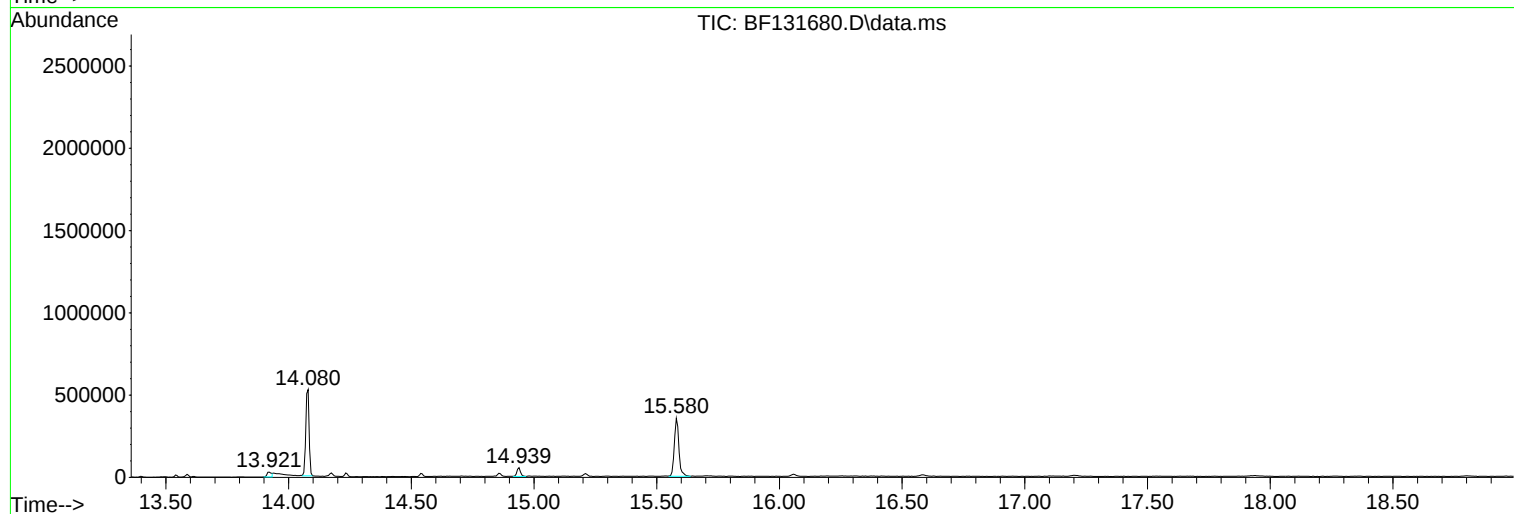
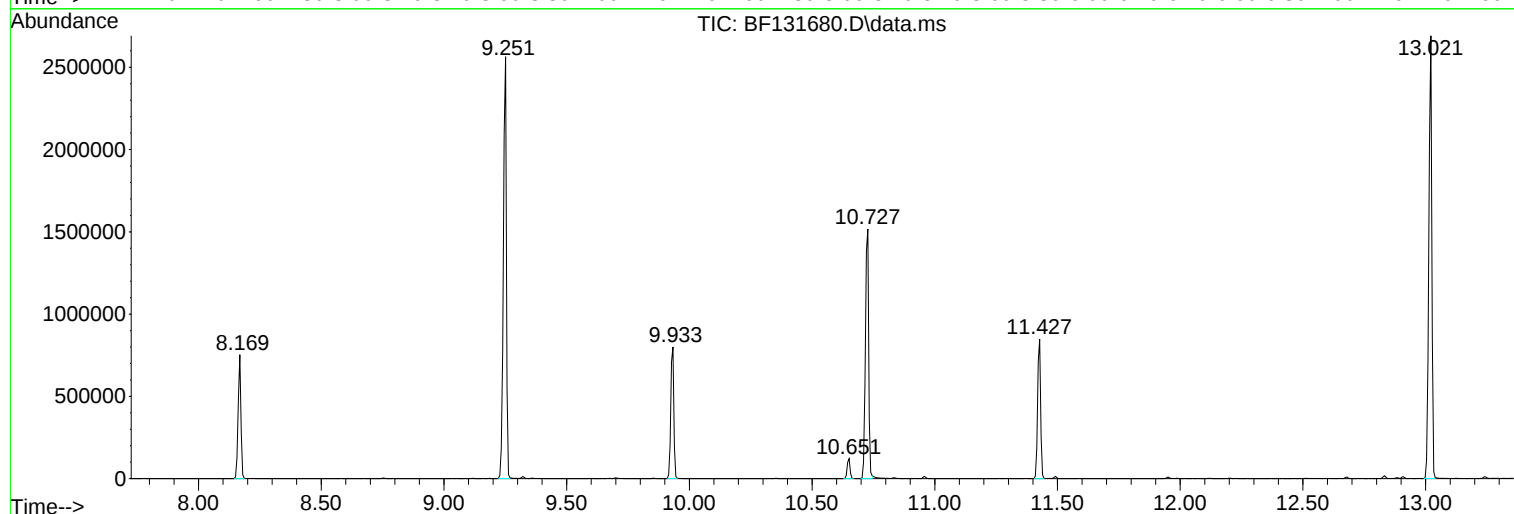
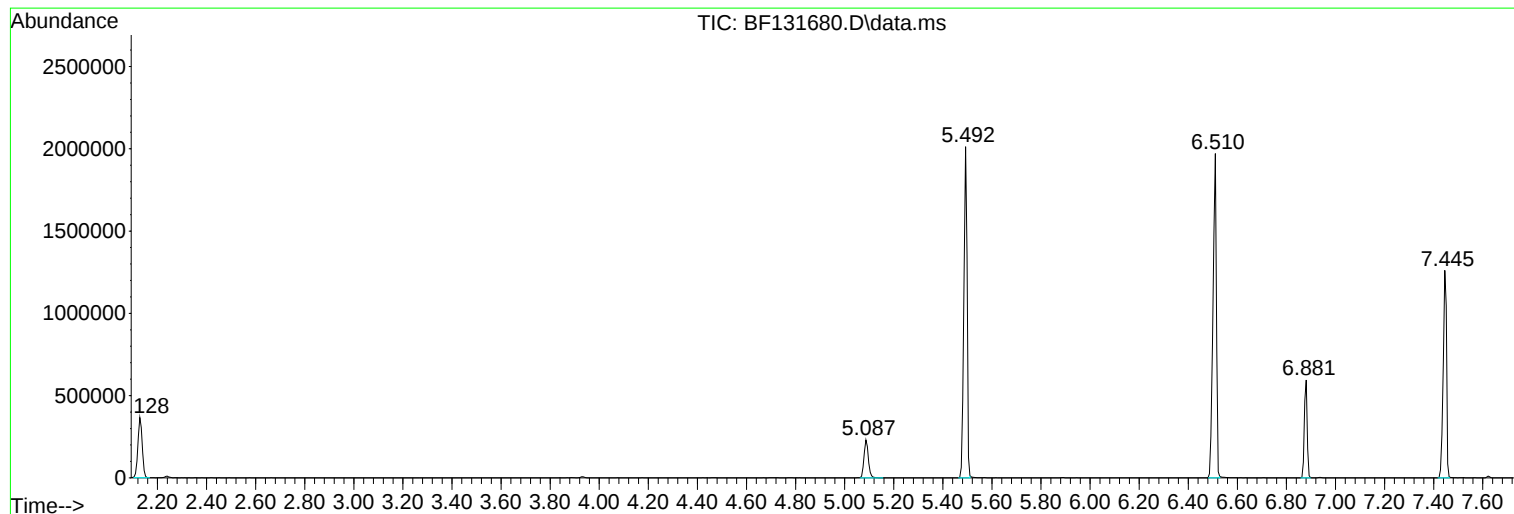
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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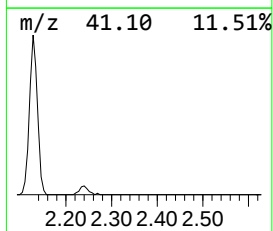
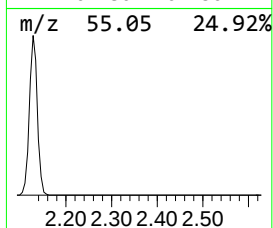
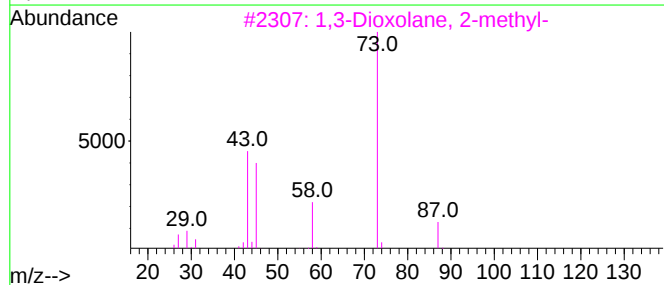
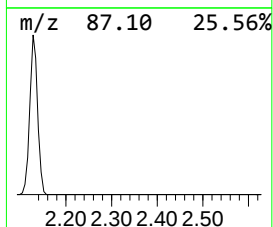
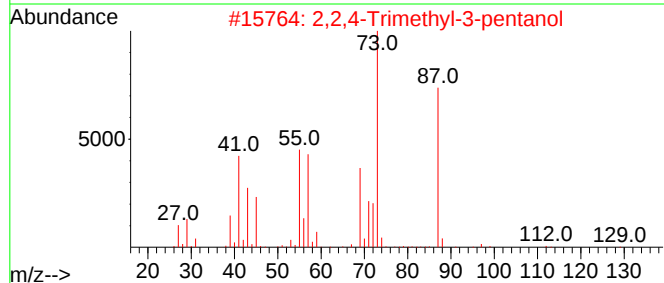
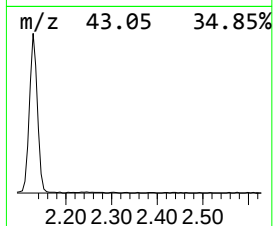
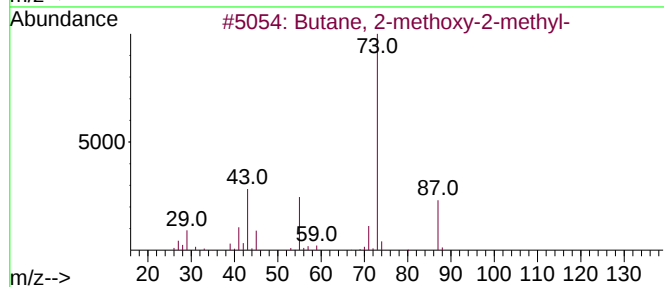
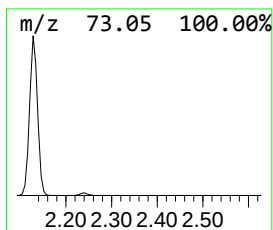
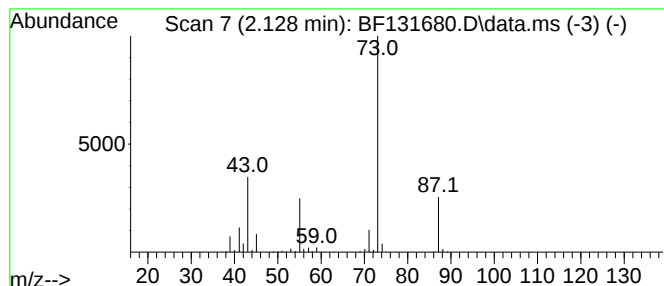
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.128	18.54 ng	442754	1,4-Dichlorobenzene-d4	6.881

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	39
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22



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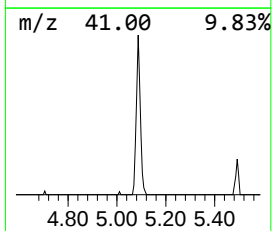
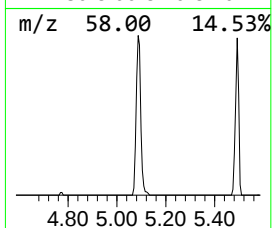
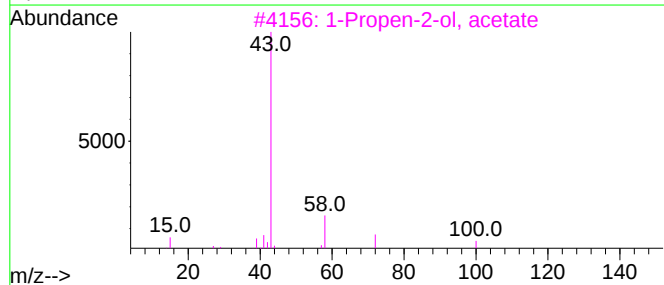
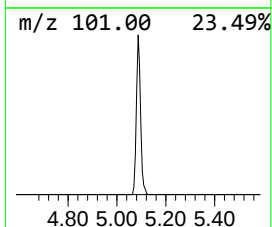
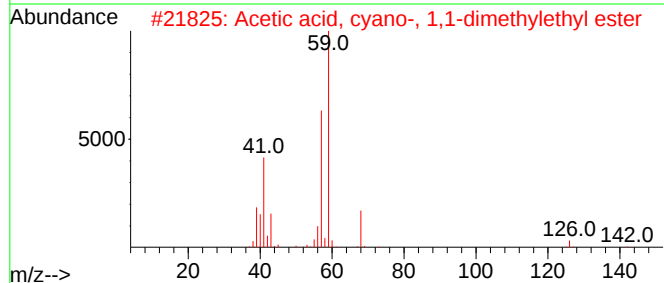
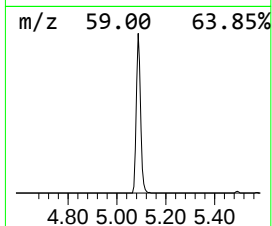
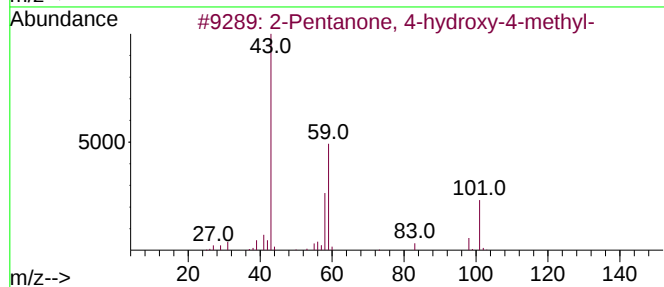
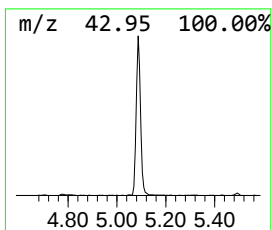
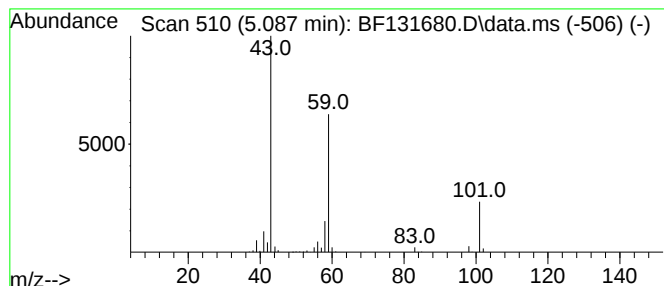
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.087	11.86 ng	283152	1,4-Dichlorobenzene-d4	6.881	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	Propanamide, N-ethyl-	101	C5H11NO	005129-72-6	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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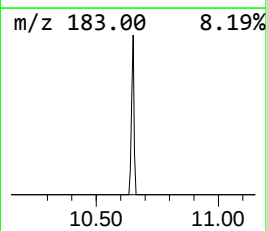
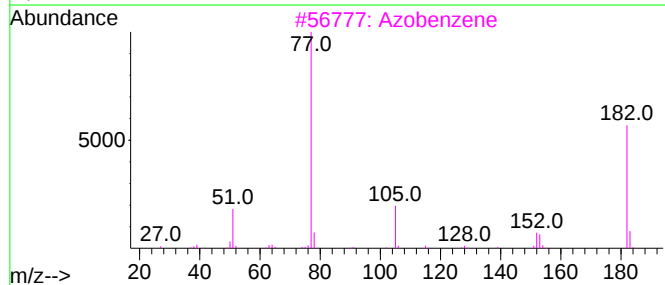
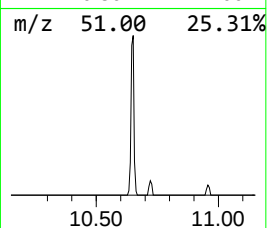
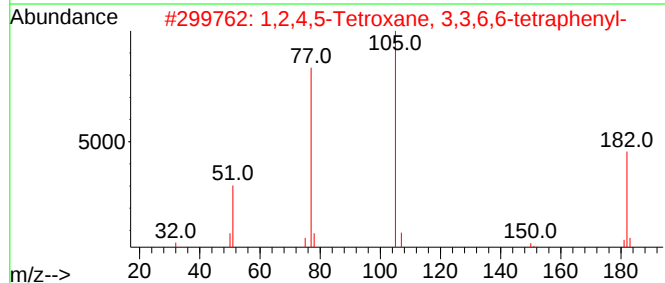
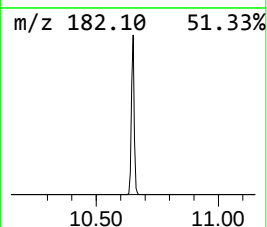
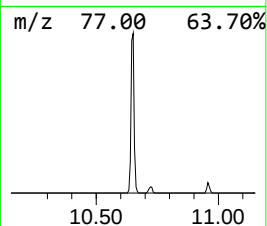
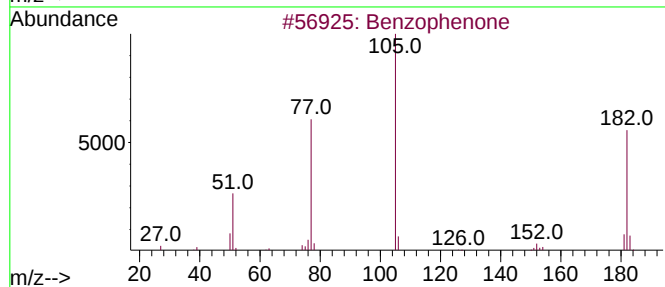
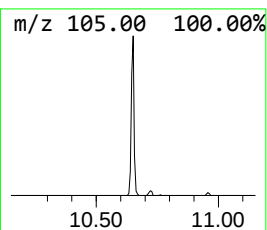
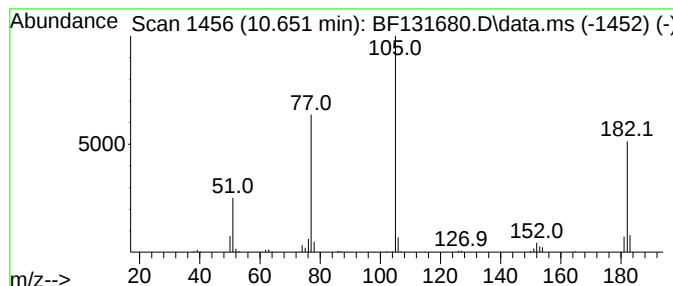
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Peak Number 3 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.651	2.83 ng	96913	Acenaphthene-d10	9.933

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	78
3			Azobenzene	182	C12H10N2	000103-33-3	59
4			1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	47
5			Phenacyl thiocyanate	177	C9H7NOS	005399-30-4	47



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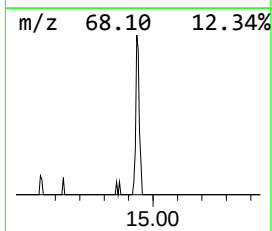
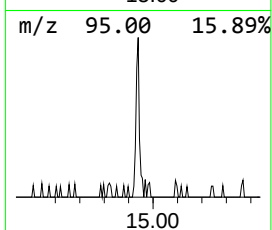
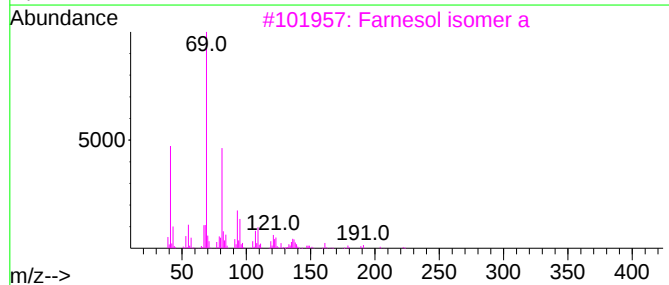
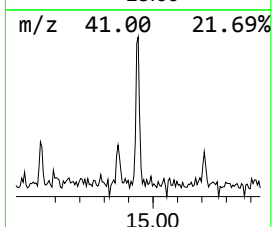
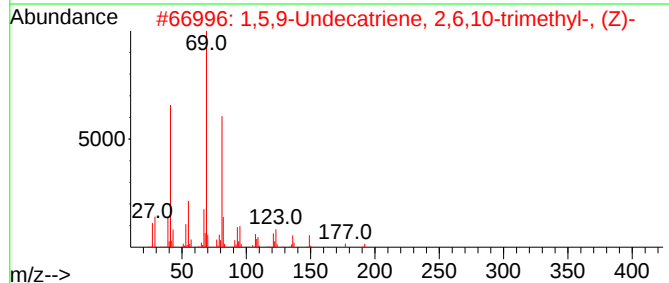
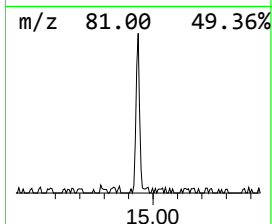
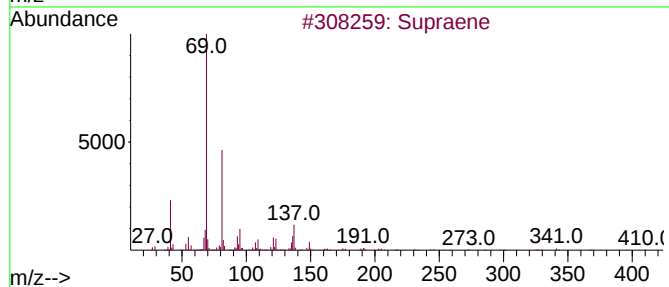
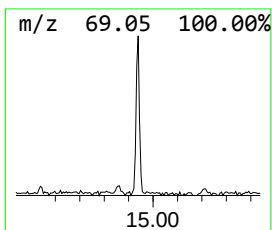
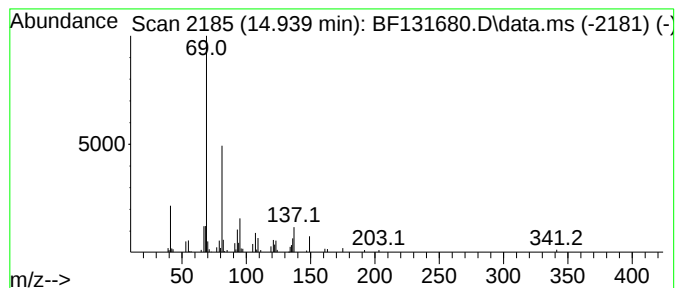
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Peak Number 4 Supraene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.939	2.33 ng	52933	Perylene-d12	15.580

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	87
2			1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	72
3			Farnesol isomer a	222	C15H26O	1000108-92-4	72
4			trans-Farnesol	222	C15H26O	000106-28-5	72
5			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.128	18.5	ng	442754	1	6.881	477633	20.0
2-Pentanone, 4-...	5.087	11.9	ng	283152	1	6.881	477633	20.0
Benzophenone	10.651	2.8	ng	96913	3	9.933	683861	20.0
Supraene	14.939	2.3	ng	52933	6	15.580	453995	20.0