

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121522\
 Data File : BF131653.D
 Acq On : 15 Dec 2022 17:19
 Operator : CG\JU
 Sample : N6038-13
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RB-35-(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: BF131653.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	15	rVB	257869	325604	24.40%	3.626%
2	4.457	399	403	409	rBV	64838	74212	5.56%	0.826%
3	5.087	504	510	513	rBV	653641	689271	51.64%	7.675%
4	5.487	575	578	588	rBV	601575	512737	38.42%	5.709%
5	6.504	747	751	754	rBV	1040255	844883	63.30%	9.408%
6	6.881	811	815	818	rBV	461419	389013	29.15%	4.332%
7	7.445	906	911	914	rBV	844986	724908	54.31%	8.072%
8	8.169	1029	1034	1037	rBV	581674	495293	37.11%	5.515%
9	9.245	1212	1217	1221	rBV	1550203	1334650	100.00%	14.862%
10	9.933	1329	1334	1337	rBV	654969	584465	43.79%	6.508%
11	10.645	1452	1455	1464	rBB	124819	93326	6.99%	1.039%
12	10.722	1464	1468	1475	rBV	178483	149898	11.23%	1.669%
13	11.427	1584	1588	1591	rBV	666658	618797	46.36%	6.890%
14	13.016	1854	1858	1862	rBV	1526786	1313667	98.43%	14.628%
15	13.851	1989	2000	2008	rBV10	15799	57317	4.29%	0.638%
16	14.074	2035	2038	2042	rBV	390113	378790	28.38%	4.218%
17	14.174	2051	2055	2059	rVB	30611	29431	2.21%	0.328%
18	14.939	2181	2185	2188	rBV	17369	16498	1.24%	0.184%
19	15.580	2289	2294	2304	rVB	279537	347802	26.06%	3.873%

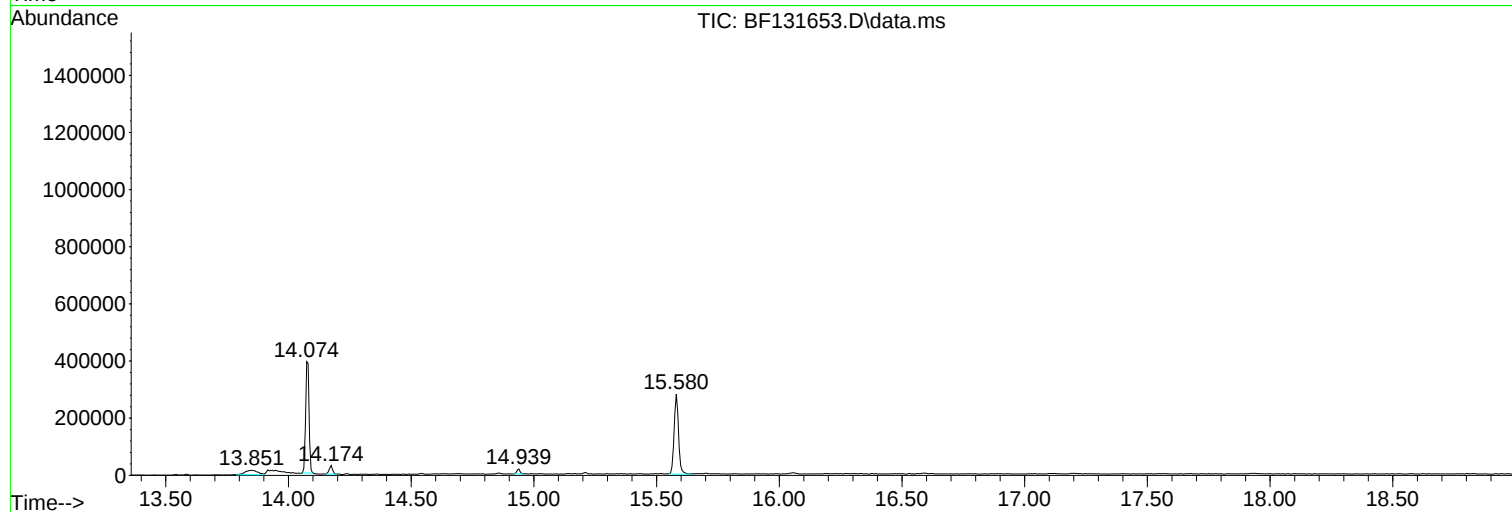
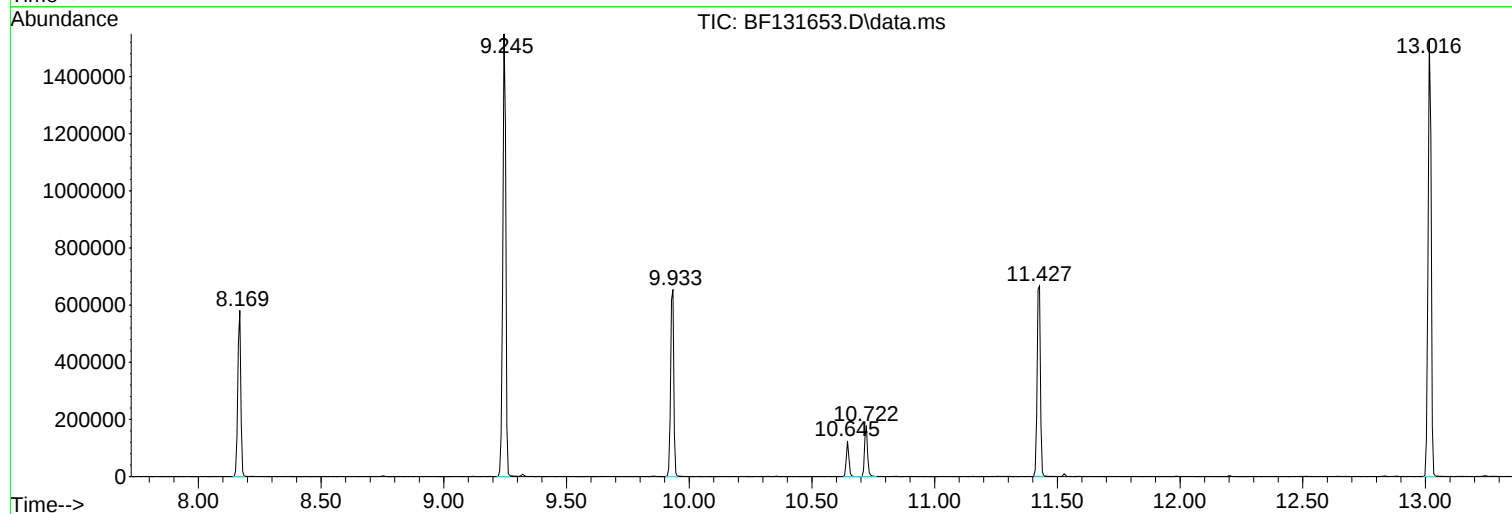
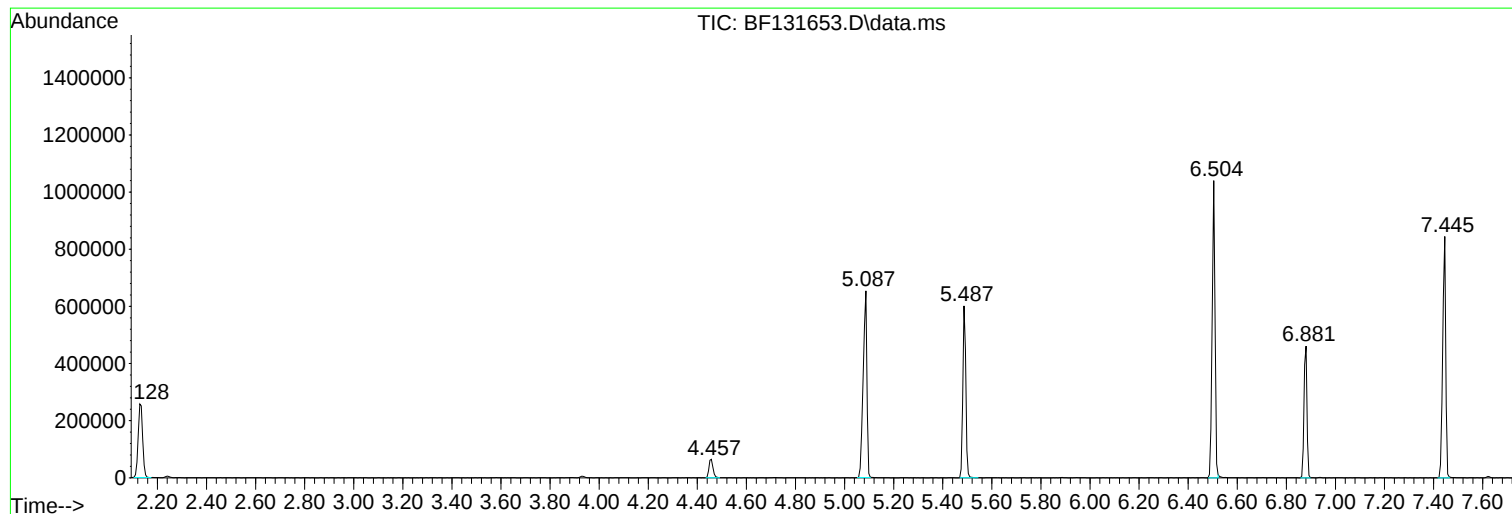
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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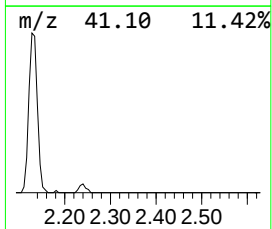
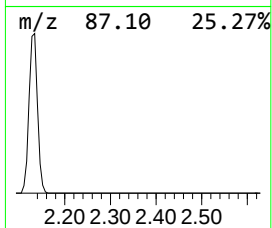
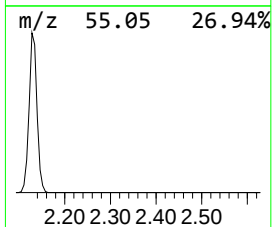
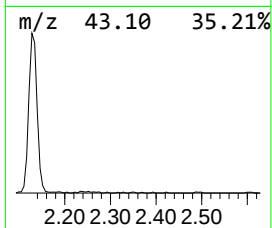
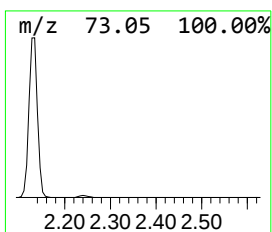
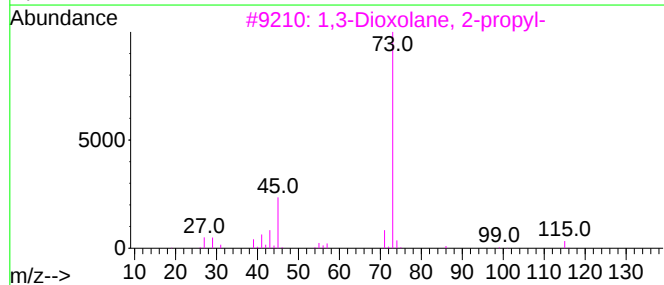
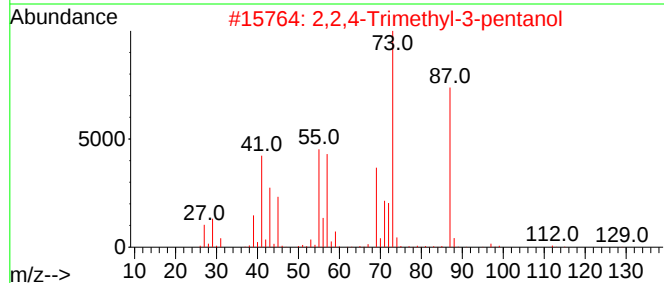
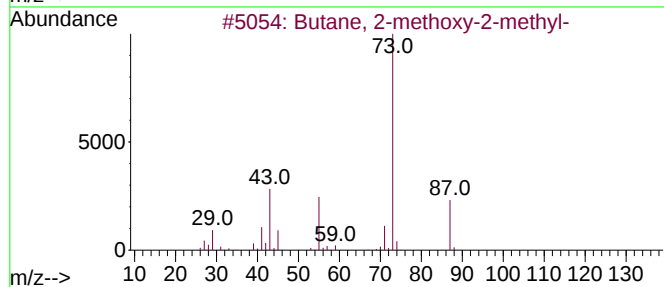
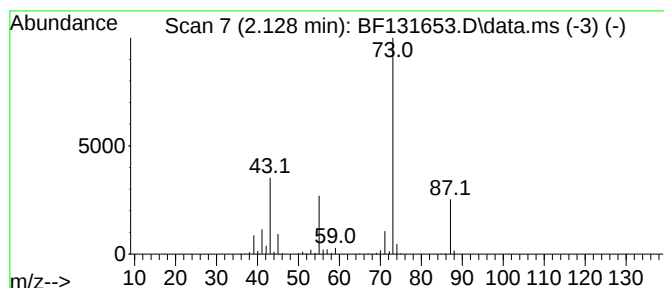
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.128	16.74 ng	325604	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	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23
4			Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	17
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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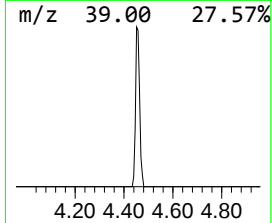
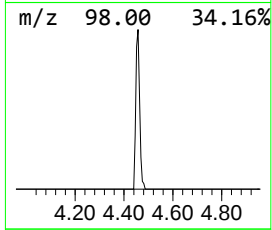
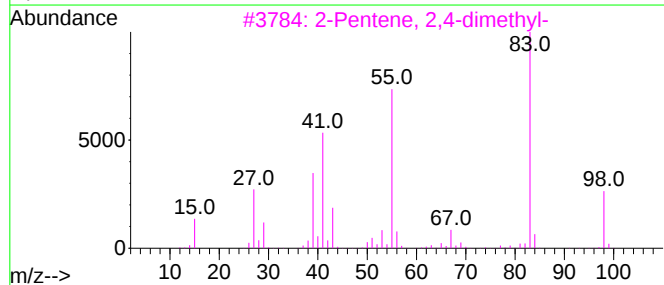
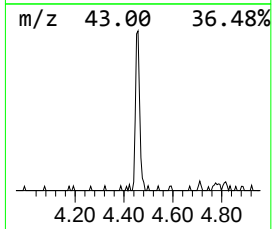
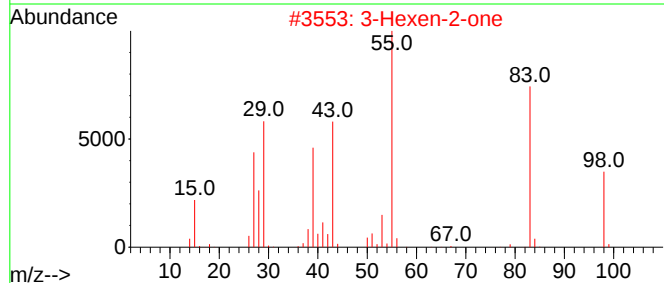
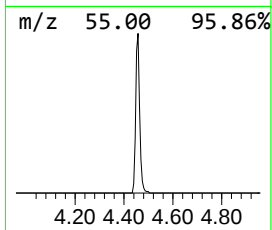
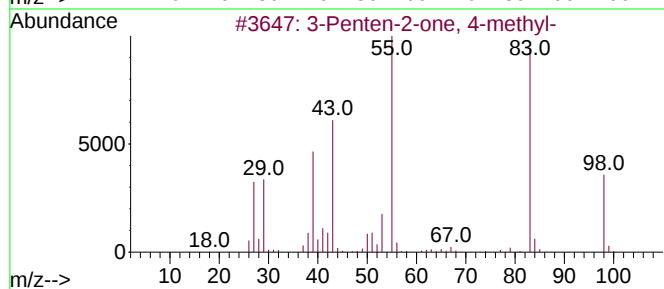
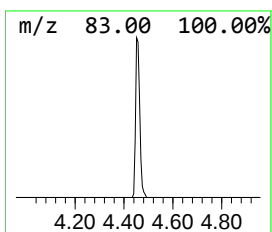
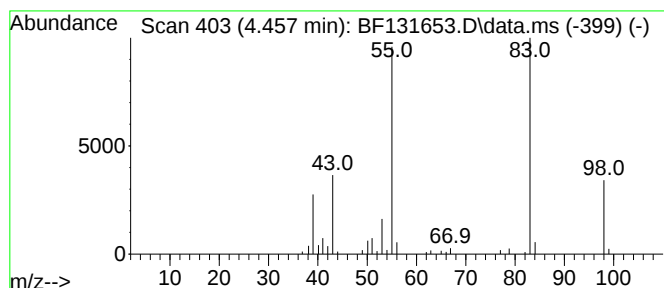
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.457	3.82 ng	74212	1,4-Dichlorobenzene-d4	6.881

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2		3-Hexen-2-one	98	C6H10O	000763-93-9	91
3		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
4		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	83
5		2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	80



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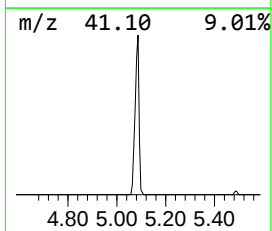
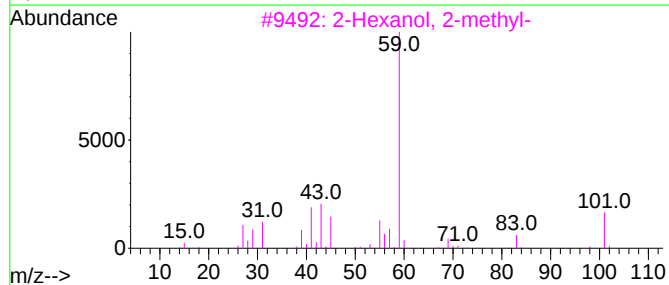
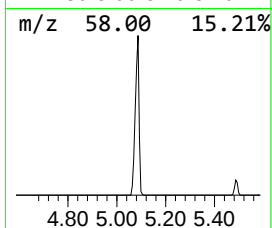
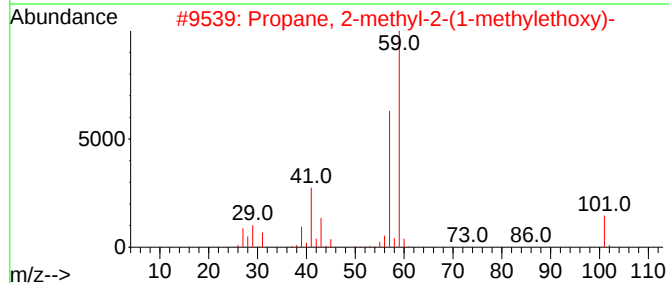
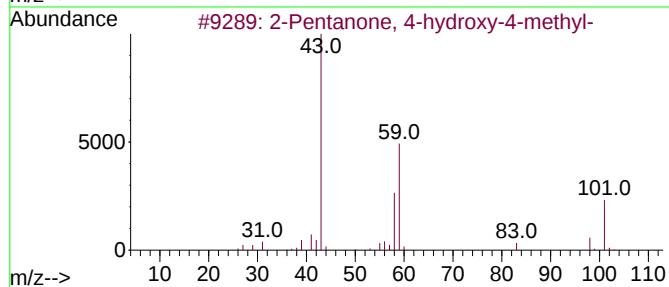
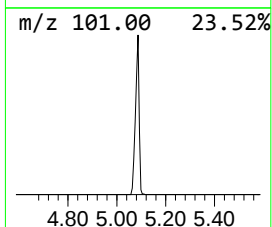
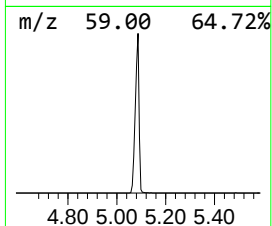
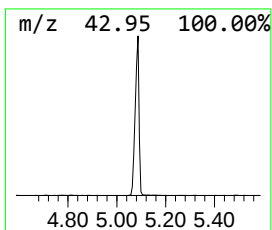
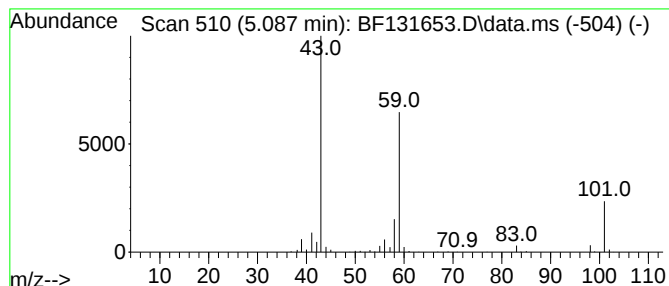
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.087	35.44 ng	689271	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			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53
3			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	40
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23



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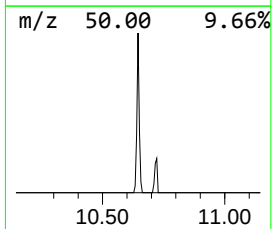
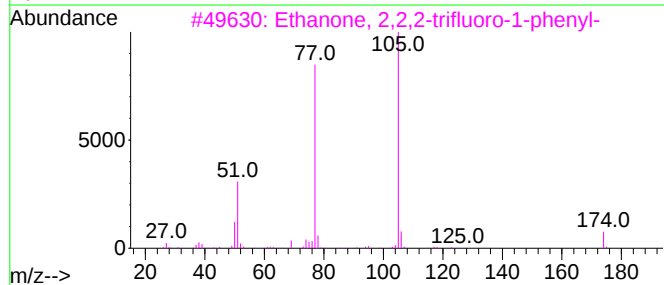
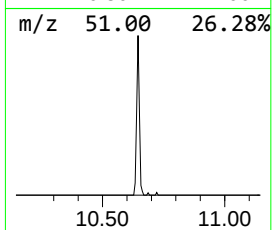
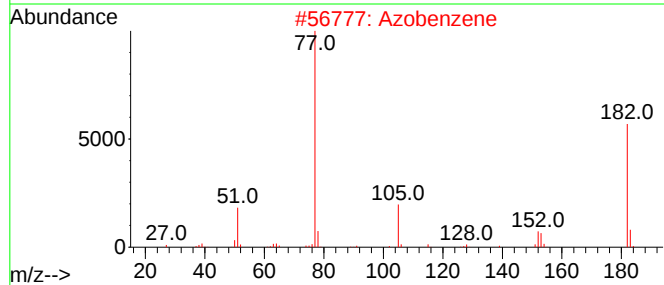
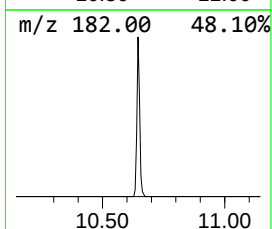
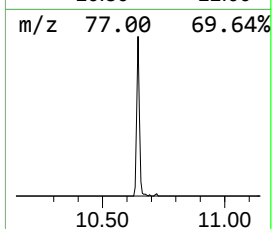
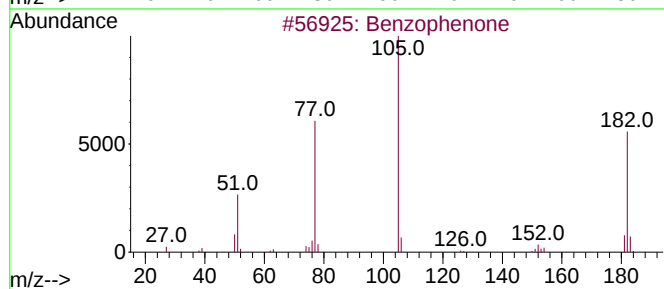
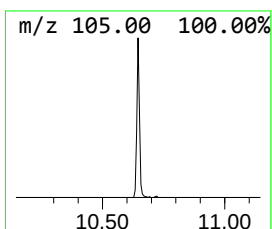
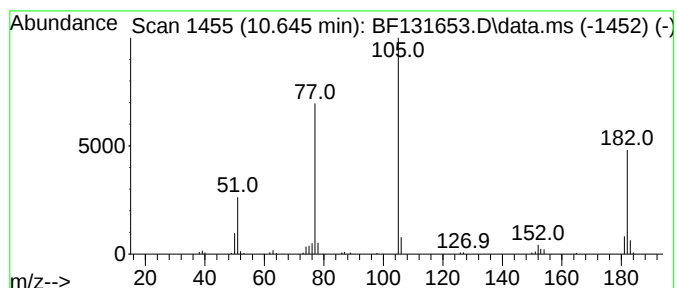
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.645	3.19 ng	93326	Acenaphthene-d10	9.933

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	95
2			Azobenzene	182	C12H10N2	000103-33-3	53
3			Ethanone, 2,2,2-trifluoro-1-phenyl-	174	C8H5F3O	000434-45-7	50
4			1,2,4-Triazine-3,5(2H,4H)-dione,...	249	C10H7N3O3S	024168-34-1	50
5			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	50



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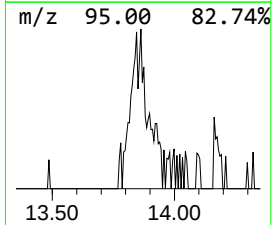
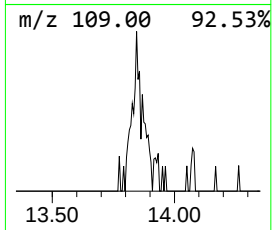
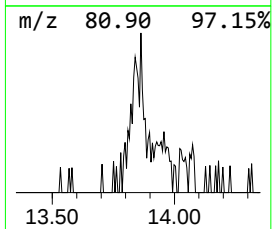
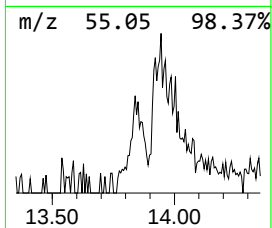
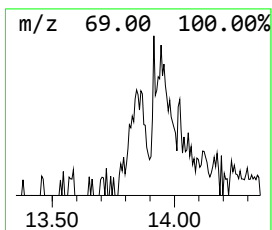
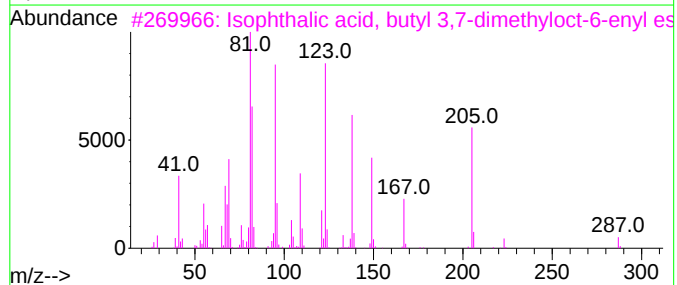
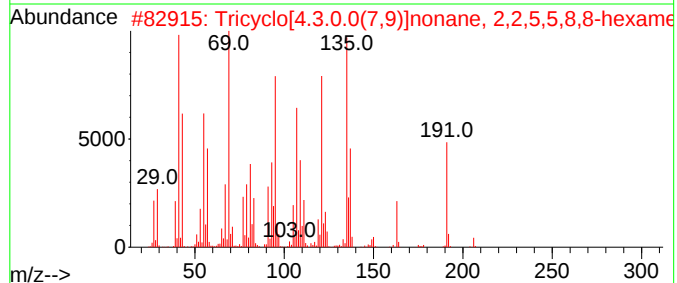
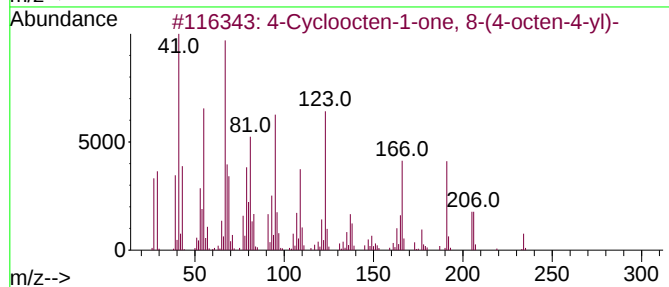
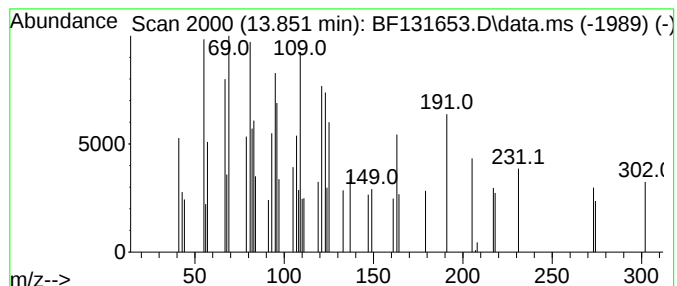
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown13.851 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.851	3.03 ng	57317	Chrysene-d12	14.074

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Cycloocten-1-one, 8-(4-octen-4-yl)-	234	C16H26O	1000152-01-9	35
2			Tricyclo[4.3.0.0(7,9)]nonane, 2,2,5,5,8,8-hexamethyl-	206	C15H26	054832-82-5	35
3			Isophthalic acid, butyl 3,7-dimethyloct-6-enyl ester	360	C22H32O4	1000356-73-8	35
4			1-Naphthalenepropanol, .alpha.-ethyl-	310	C20H38O	057397-30-5	30
5			Longifolenaldehyde	220	C15H24O	019890-84-7	30



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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	16.7	ng	325604	1	6.881	389013	20.0
3-Penten-2-one,...	4.457	3.8	ng	74212	1	6.881	389013	20.0
2-Pentanone, 4-...	5.087	35.4	ng	689271	1	6.881	389013	20.0
Benzophenone	10.645	3.2	ng	93326	3	9.933	584465	20.0
unknown13.851	13.851	3.0	ng	57317	5	14.074	378790	20.0