

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121522\
 Data File : BF131657.D
 Acq On : 15 Dec 2022 19:30
 Operator : CG\JU
 Sample : N6038-10
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RB-33-(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: BF131657.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.140	3	9	15	rVB	409704	495138	23.18%	3.352%
2	4.457	399	403	410	rVB	86591	97372	4.56%	0.659%
3	5.093	506	511	520	rVB	378894	491606	23.02%	3.328%
4	5.498	575	580	583	rBV	1747937	1764314	82.60%	11.943%
5	6.510	747	752	755	rBV	1864361	1890029	88.48%	12.794%
6	6.881	811	815	818	rBV	547526	442118	20.70%	2.993%
7	7.445	906	911	914	rBV	1263025	1216604	56.96%	8.236%
8	8.169	1030	1034	1037	rBV	659277	553893	25.93%	3.750%
9	9.251	1212	1218	1221	rBV	2433608	2135994	100.00%	14.459%
10	9.933	1329	1334	1337	rBV	797711	662416	31.01%	4.484%
11	10.651	1452	1456	1459	rBV	116512	94785	4.44%	0.642%
12	10.728	1464	1469	1472	rBV	1227383	1127107	52.77%	7.630%
13	11.428	1584	1588	1591	rBV	825536	701660	32.85%	4.750%
14	11.527	1602	1605	1608	rBV2	29149	23646	1.11%	0.160%
15	12.645	1792	1795	1798	rVB	52176	44064	2.06%	0.298%
16	12.874	1829	1834	1838	rVB	49833	48724	2.28%	0.330%
17	13.022	1854	1859	1862	rBV	2243695	1863665	87.25%	12.616%
18	13.921	2008	2012	2031	rBV3	53422	181039	8.48%	1.226%
19	14.080	2034	2039	2042	rBV	438181	423607	19.83%	2.868%
20	14.174	2050	2055	2060	rVB	35766	42250	1.98%	0.286%
21	15.133	2214	2218	2222	rBV	16459	26284	1.23%	0.178%
22	15.510	2278	2282	2289	rBV	15460	24204	1.13%	0.164%
23	15.580	2289	2294	2303	rVV	333626	421845	19.75%	2.856%

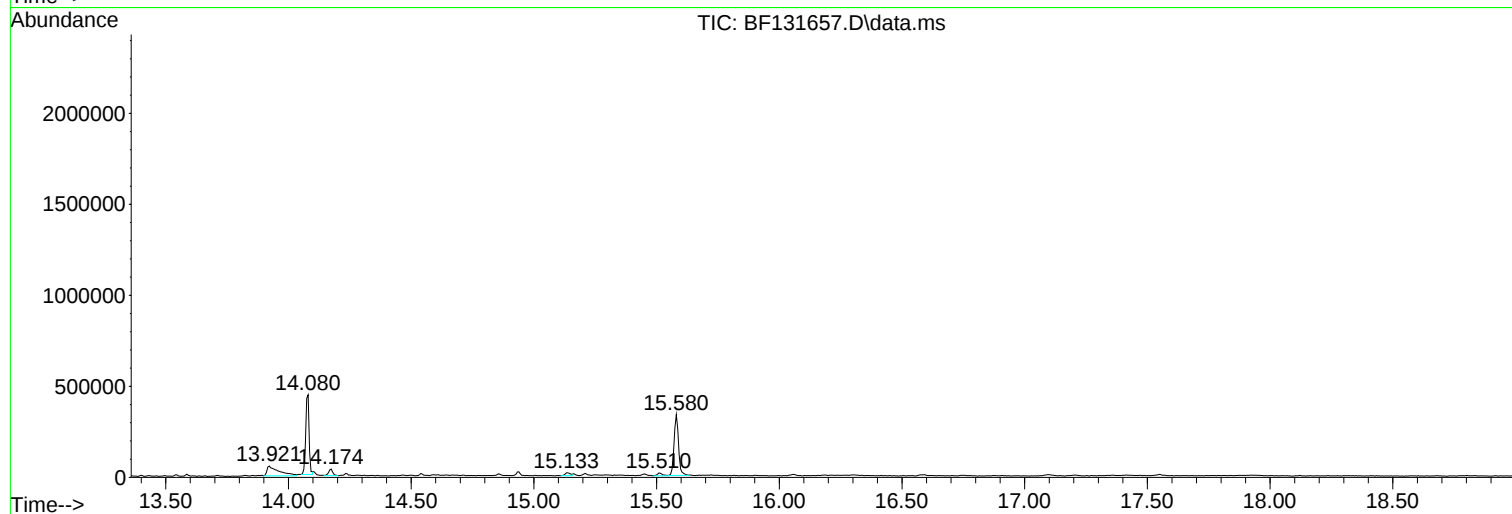
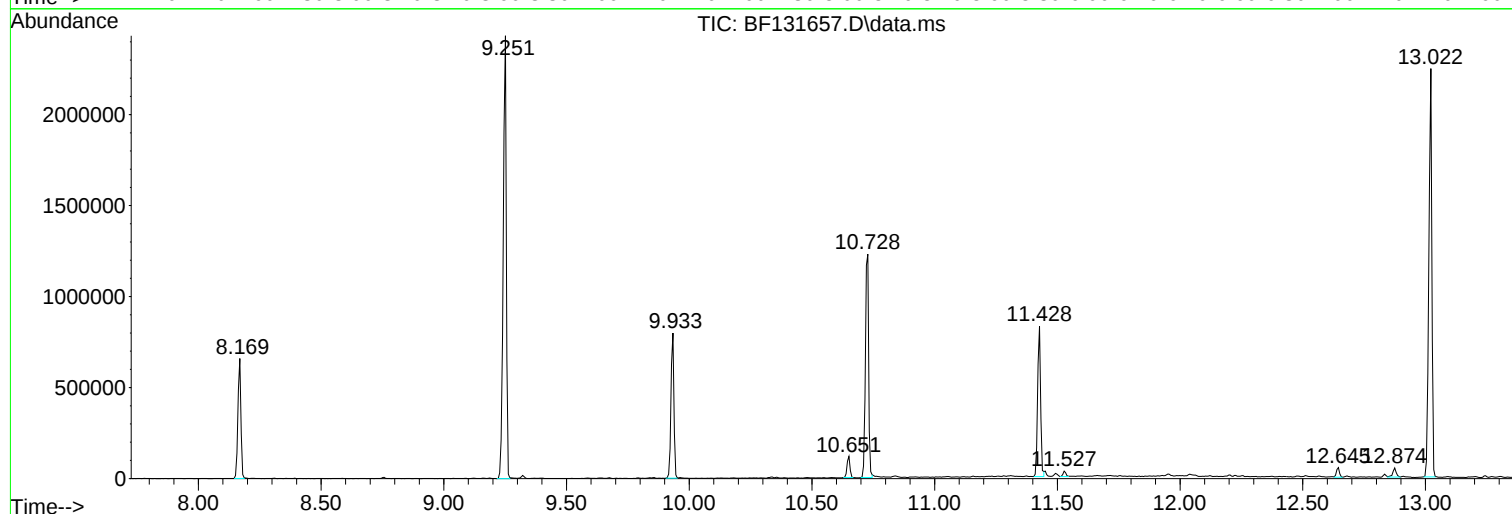
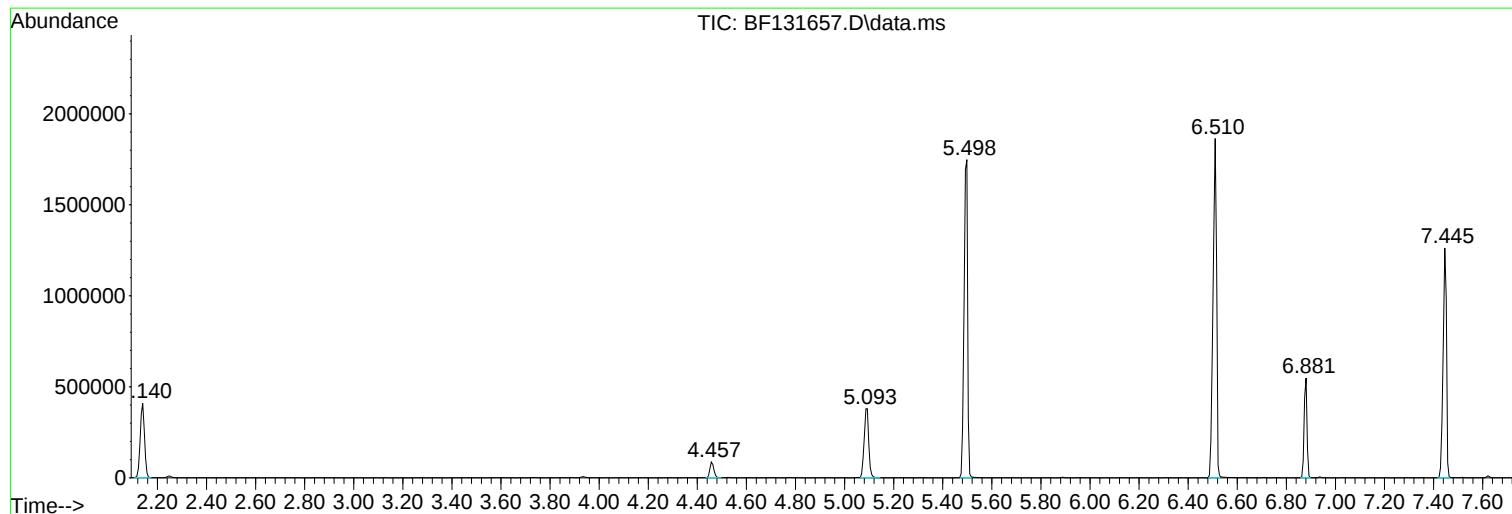
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ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RB-33-(5-7)

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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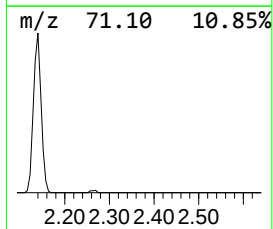
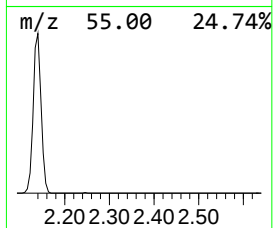
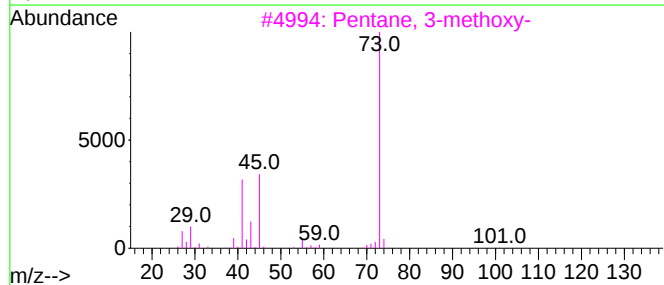
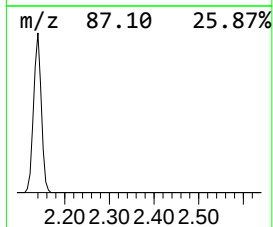
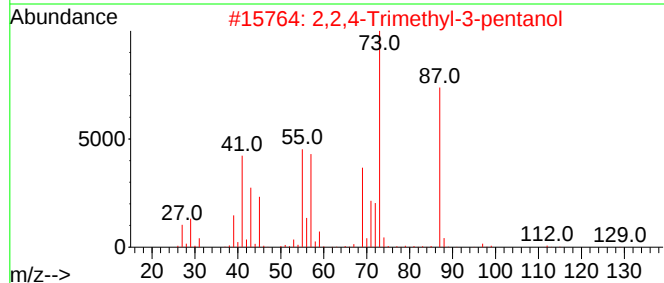
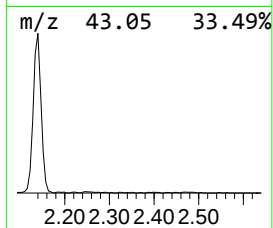
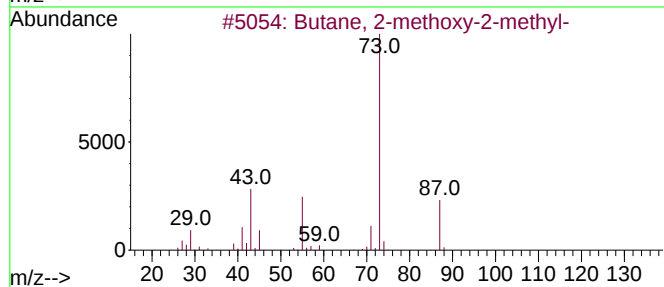
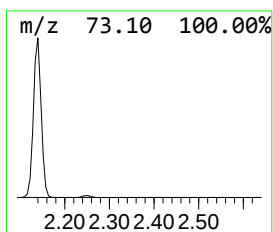
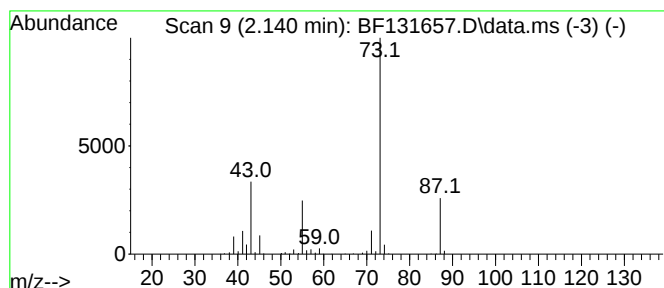
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.140	22.40 ng	495138	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			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
5			N-Ethylformamide	73	C3H7NO	000627-45-2	9



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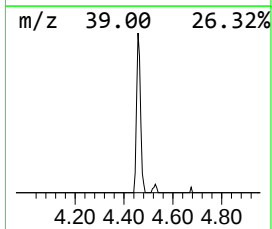
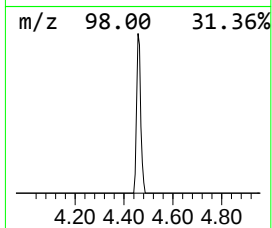
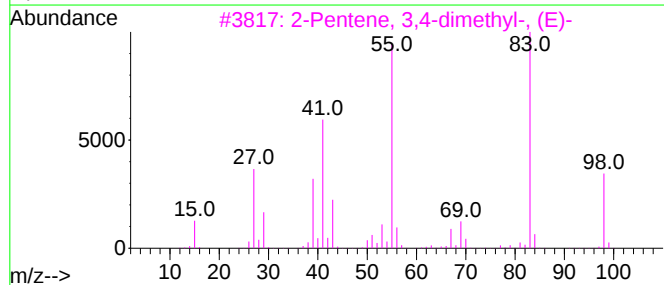
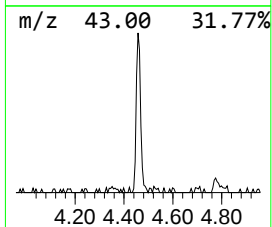
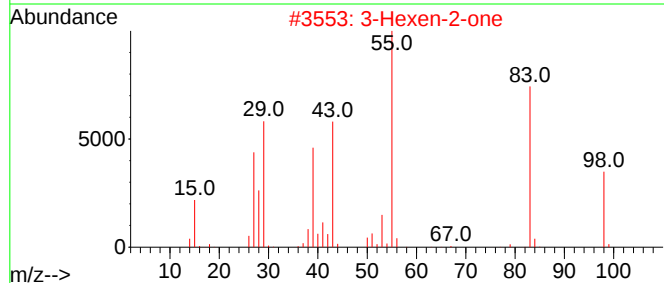
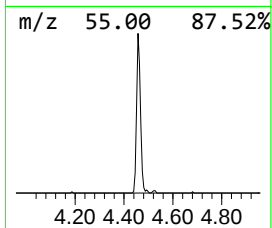
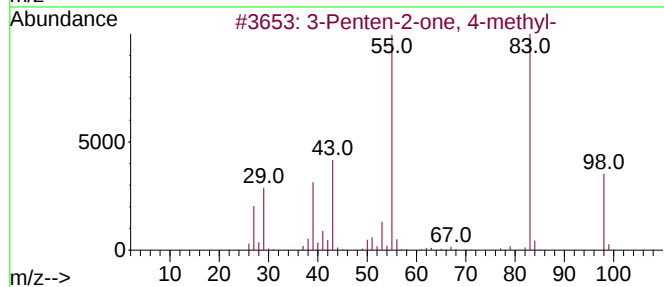
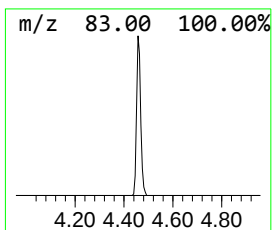
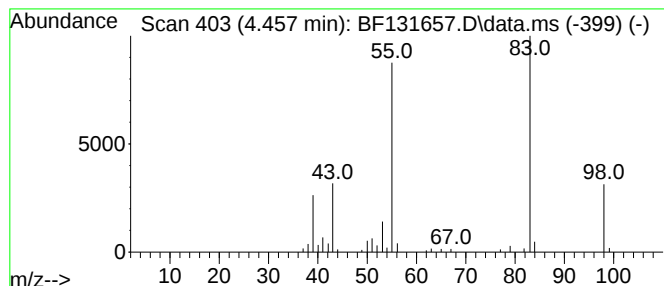
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.457	4.40 ng	97372	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, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
5		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86



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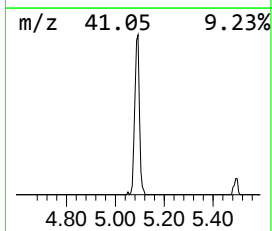
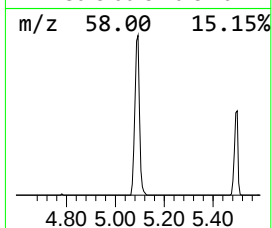
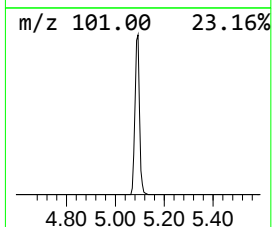
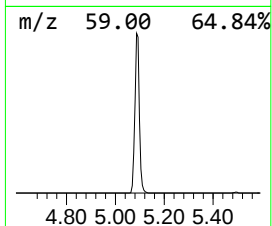
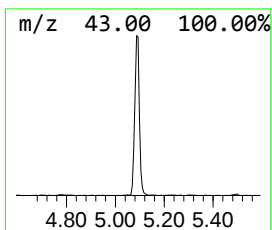
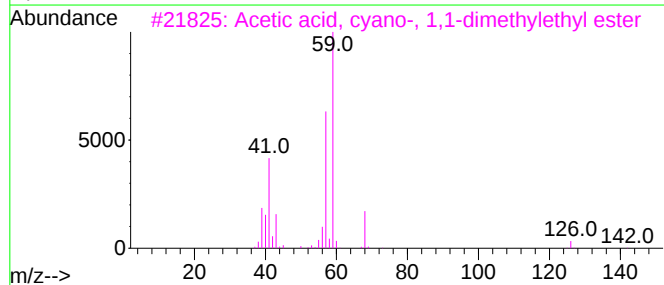
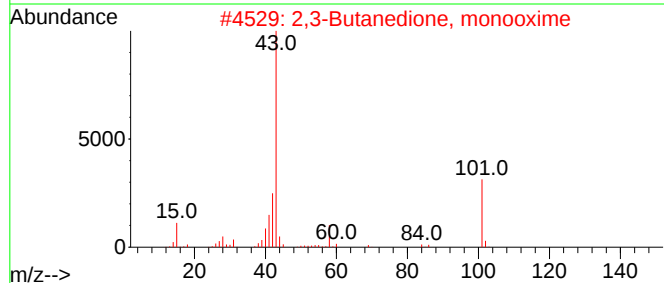
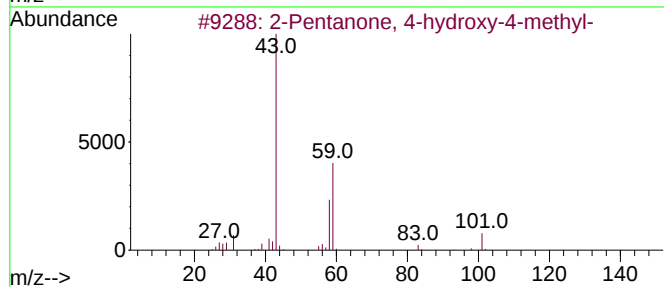
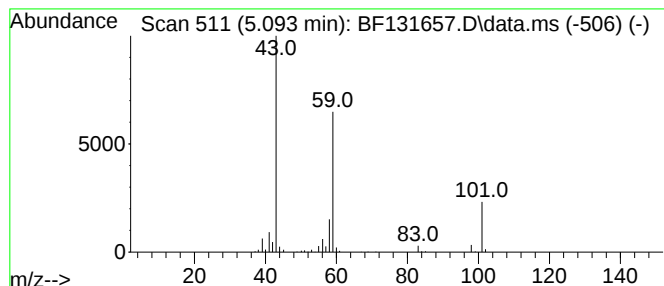
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.093	22.24 ng	491606	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			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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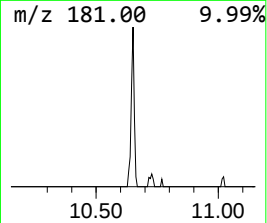
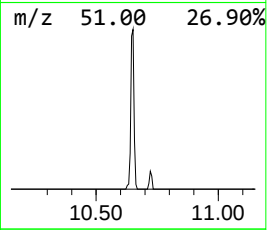
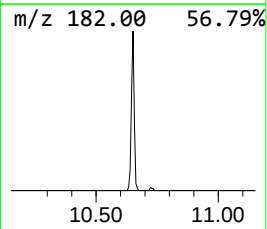
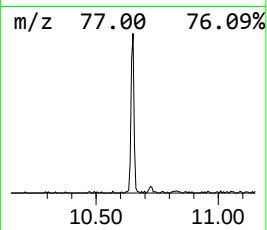
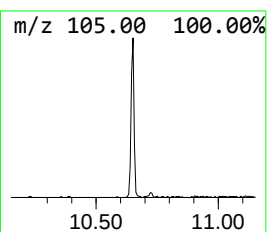
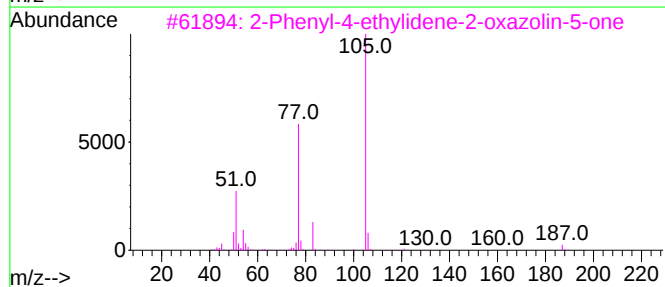
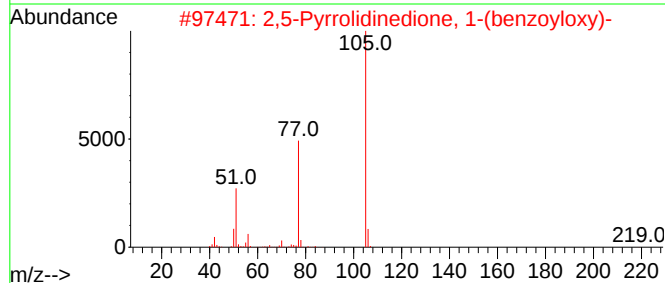
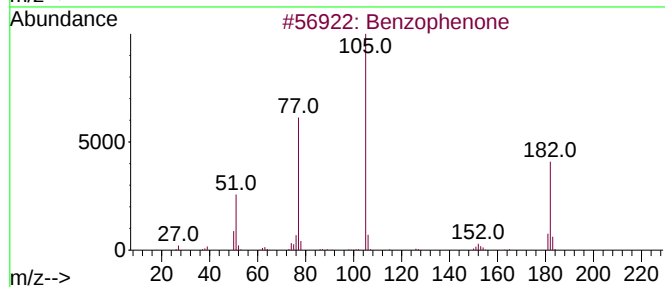
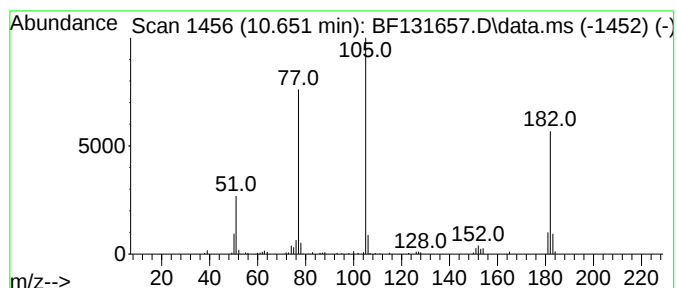
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.651	2.86 ng	94785	Acenaphthene-d10	9.933

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			2,5-Pyrrolidinedione, 1-(benzoyl...	219	C11H9NO4	023405-15-4	50
3			2-Phenyl-4-ethylidene-2-oxazolin...	187	C11H9NO2	037791-41-6	50
4			Disulfide, dibenzoyl	274	C14H10O2S2	000644-32-6	50
5			Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	50



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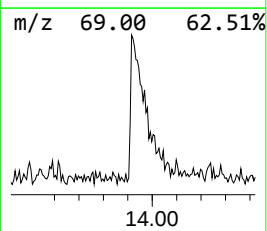
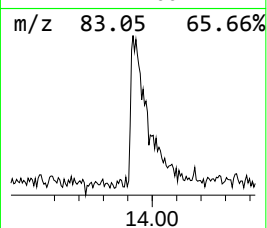
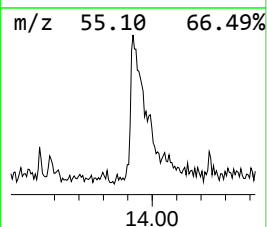
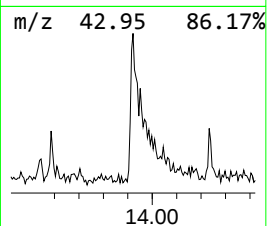
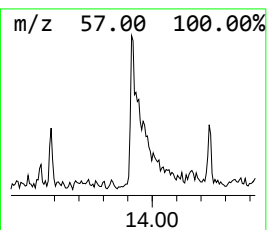
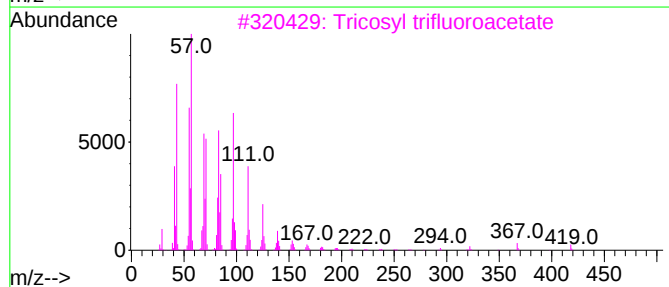
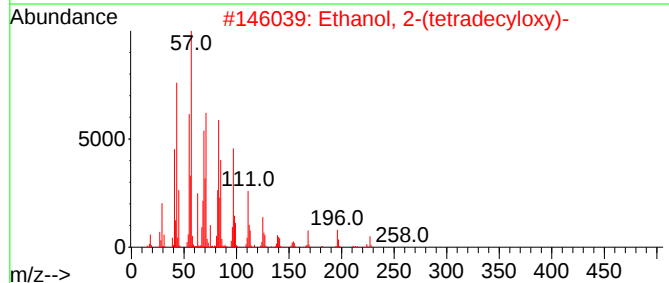
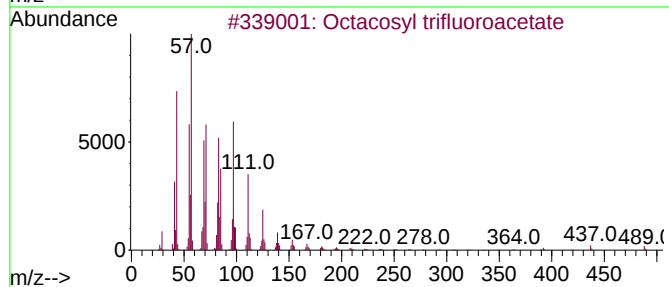
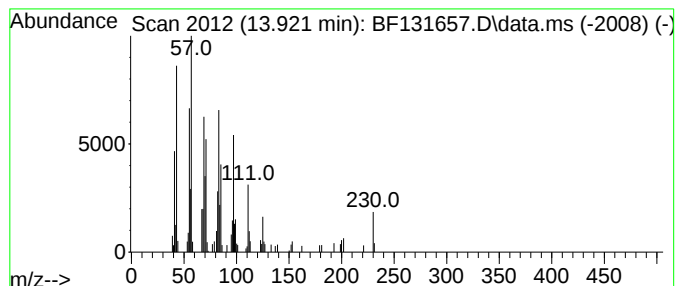
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Octacosyl trifluoroacetate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.922	8.55 ng	181039	Chrysene-d12	14.080

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	93
2			Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
3			Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	91
4			Tricosyl pentafluoropropionate	486	C26H47F5O2	1000351-81-0	90
5			Tricosyl heptafluorobutyrate	536	C27H47F7O2	1000351-83-4	90



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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...	2.140	22.4	ng	495138	1	6.881	442118	20.0
3-Penten-2-one,...	4.457	4.4	ng	97372	1	6.881	442118	20.0
2-Pentanone, 4-...	5.093	22.2	ng	491606	1	6.881	442118	20.0
Benzophenone	10.651	2.9	ng	94785	3	9.933	662416	20.0
Octacosyl trifl...	13.922	8.6	ng	181039	5	14.080	423607	20.0