

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112024\
 Data File : BF140493.D
 Acq On : 20 Nov 2024 11:49
 Operator : RC/JU
 Sample : P4868-01
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RW5-SP100-20241114

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-BF111324.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF140493.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	8	22	rVB	2365519	3732743	60.67%	11.462%
2	2.522	58	73	89	rBV	3199880	6152621	100.00%	18.893%
3	2.646	89	94	104	rVB	46847	81540	1.33%	0.250%
4	4.475	399	405	420	rBV	175466	264967	4.31%	0.814%
5	5.087	500	509	522	rBV	133091	203696	3.31%	0.625%
6	5.504	574	580	599	rBV	1222391	1632755	26.54%	5.014%
7	6.510	740	751	760	rBV	774774	1051570	17.09%	3.229%
8	6.875	807	813	818	rBV	534388	679502	11.04%	2.087%
9	7.433	902	908	918	rBV	1797441	2492504	40.51%	7.654%
10	8.151	1022	1030	1047	rBV	679734	894917	14.55%	2.748%
11	9.227	1207	1213	1218	rBV	3471017	4499754	73.14%	13.817%
12	9.910	1323	1329	1347	rBV	794846	1039111	16.89%	3.191%
13	10.704	1458	1464	1480	rBV	2096297	2927152	47.58%	8.988%
14	11.398	1577	1582	1596	rBV	854626	1094921	17.80%	3.362%
15	12.986	1846	1852	1857	rBV	3337103	4437251	72.12%	13.626%
16	14.051	2027	2033	2042	rBV	567325	773814	12.58%	2.376%
17	15.556	2283	2289	2305	rVB	361165	606799	9.86%	1.863%

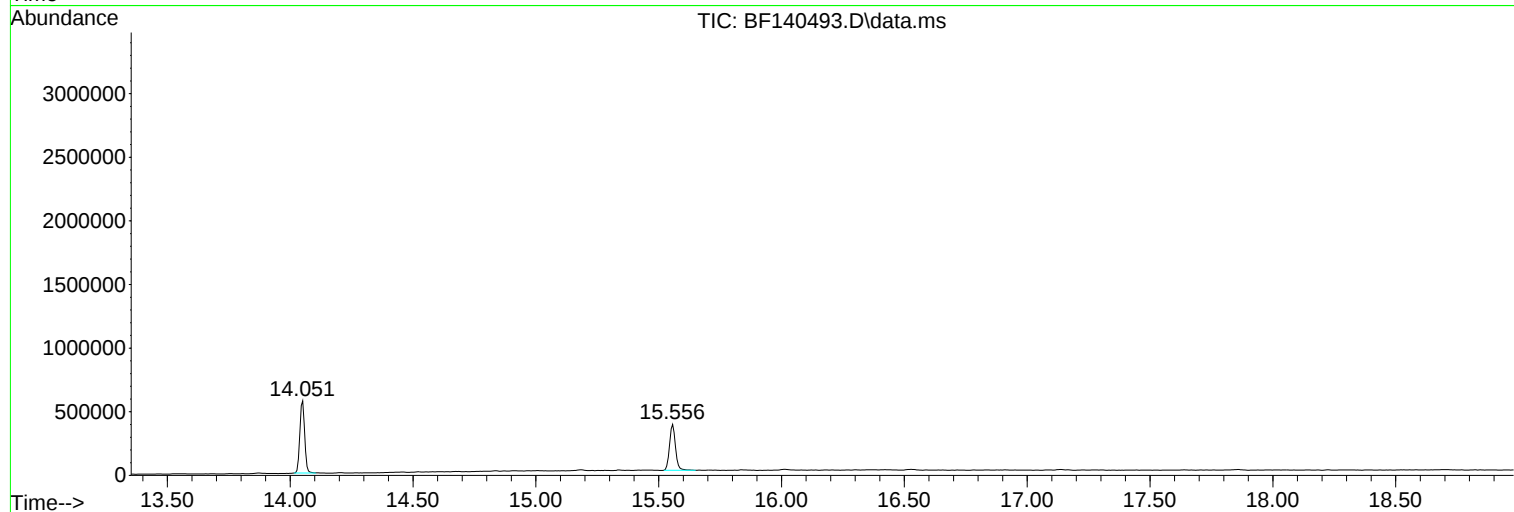
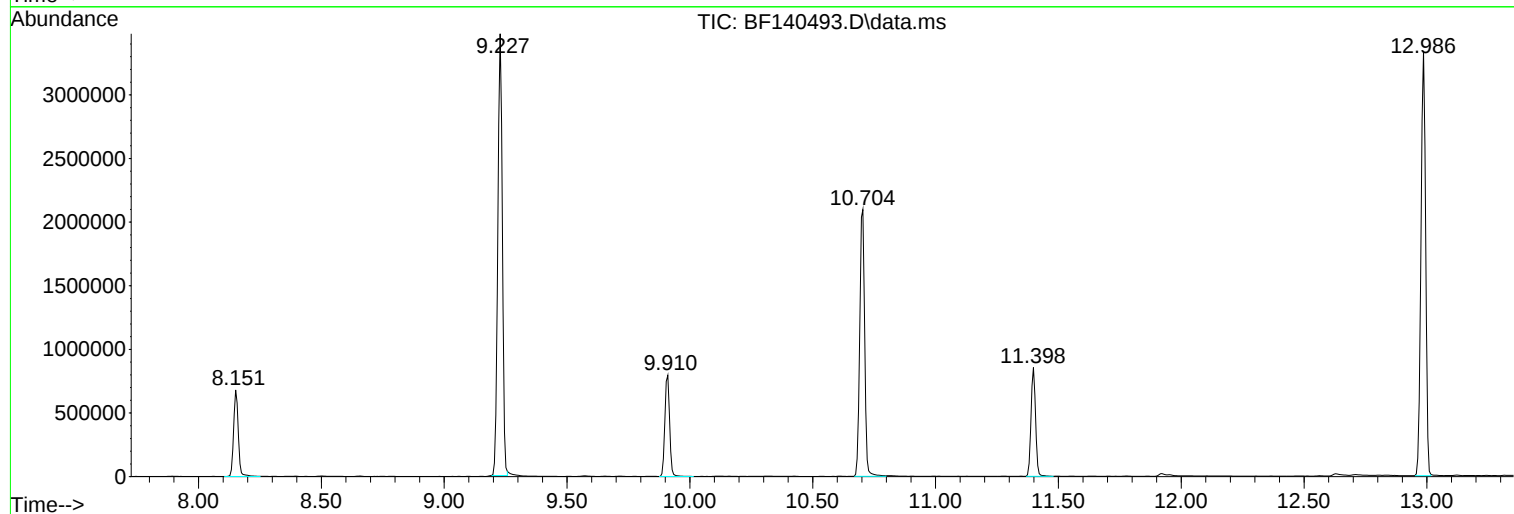
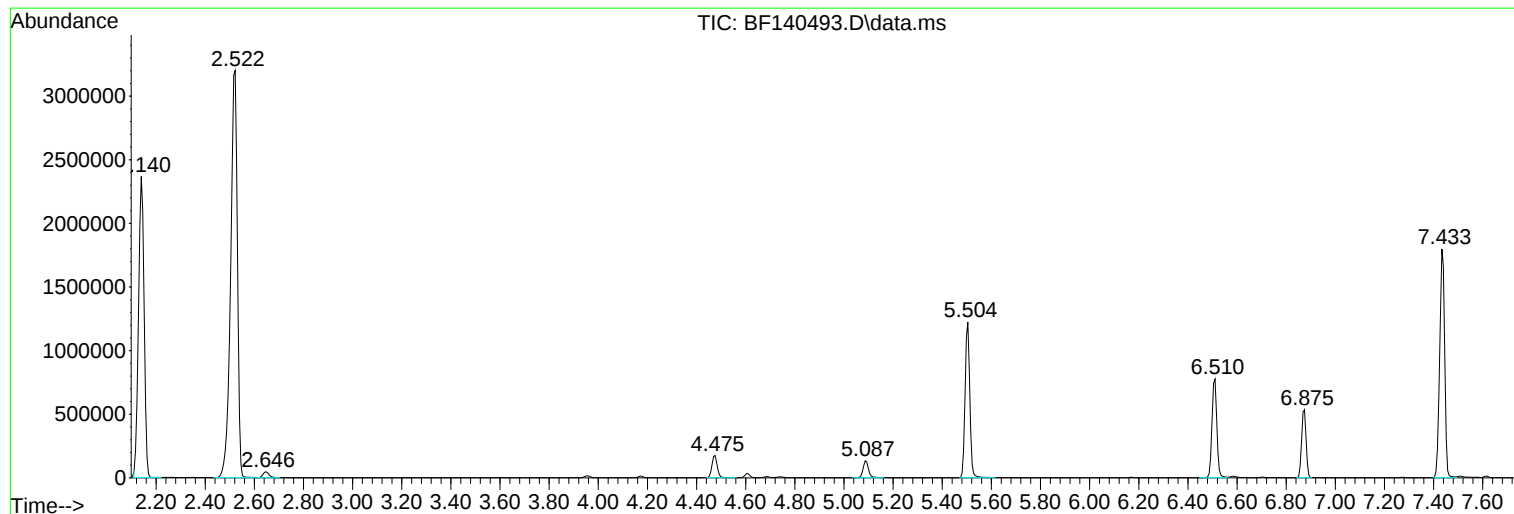
Sum of corrected areas: 32565617

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111324.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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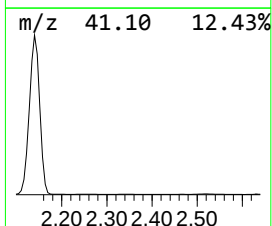
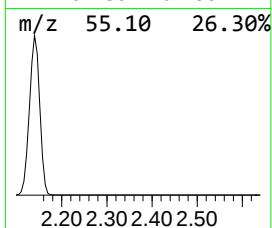
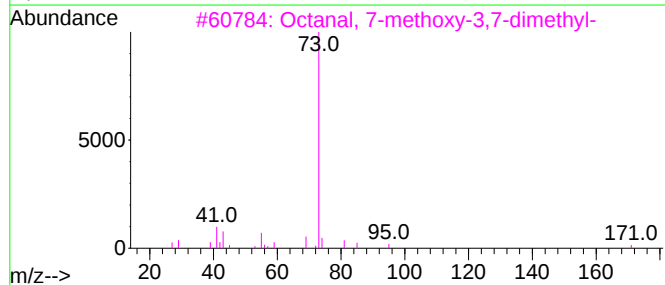
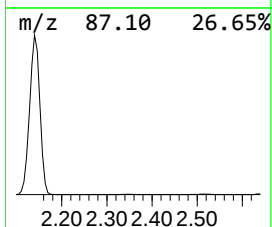
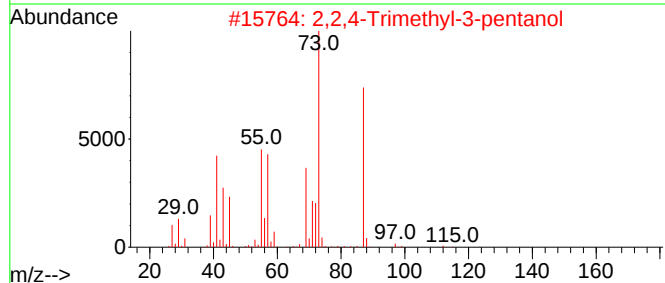
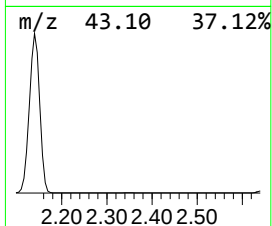
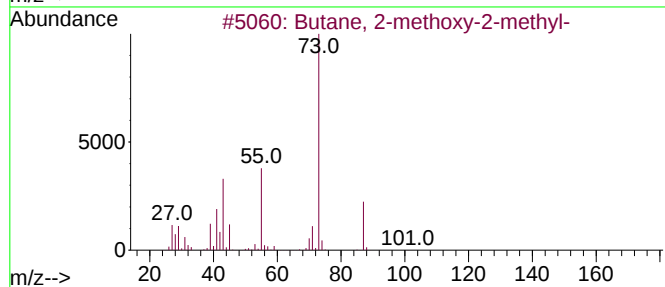
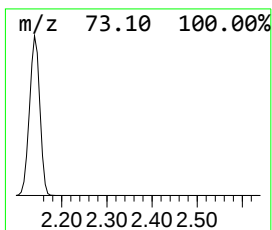
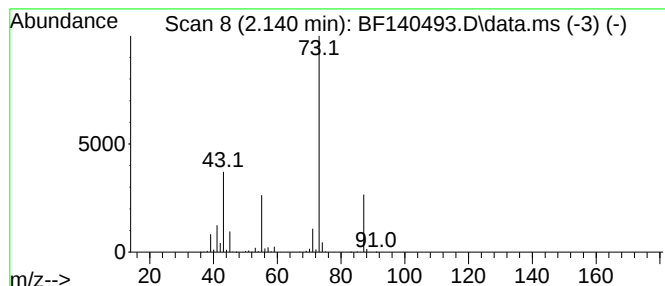
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.140	109.87 ng	3732740	1,4-Dichlorobenzene-d4	6.875

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			Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	23
4			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17



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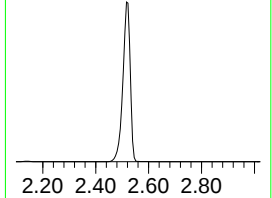
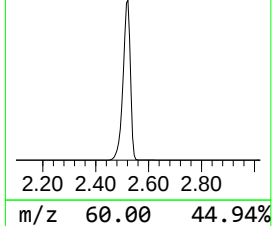
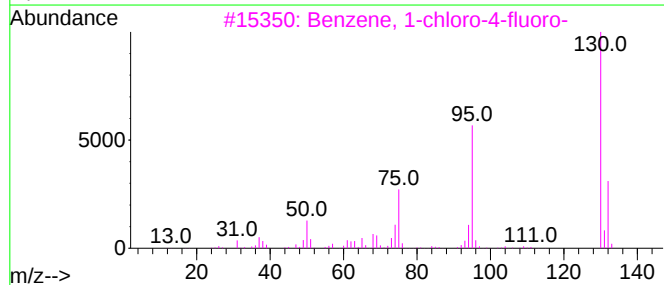
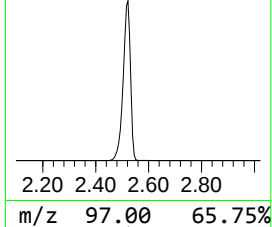
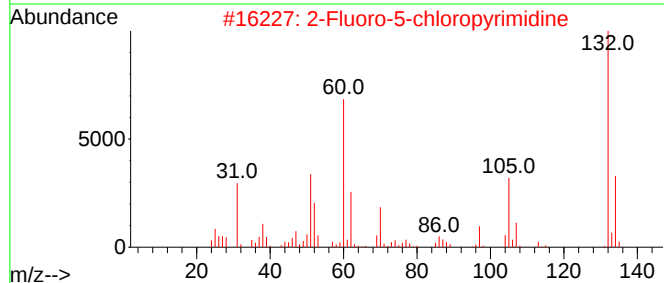
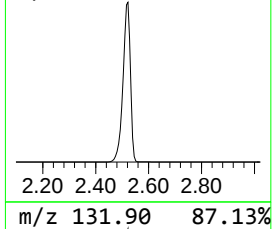
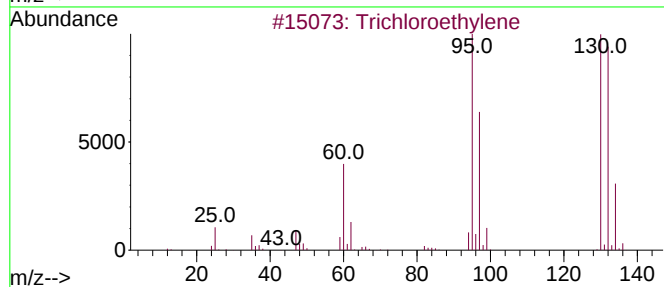
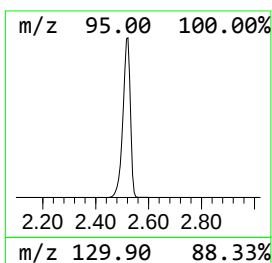
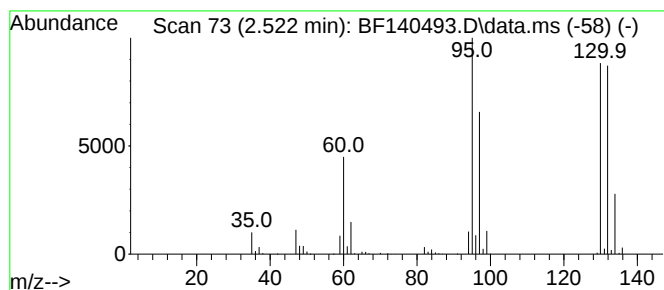
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Trichloroethylene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.522	181.09 ng	6152620	1,4-Dichlorobenzene-d4	6.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trichloroethylene	130	C2HCl3	000079-01-6	99
2			2-Fluoro-5-chloropyrimidine	132	C4H2ClFN2	062802-37-3	35
3			Benzene, 1-chloro-4-fluoro-	130	C6H4ClF	000352-33-0	14
4			Butylthiourea	132	C5H12N2S	001516-32-1	10
5			Isoquinoline, 3,4-dihydro-	131	C9H9N	003230-65-7	10



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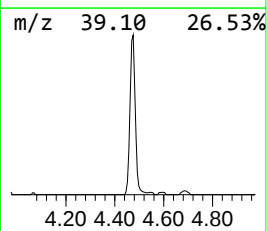
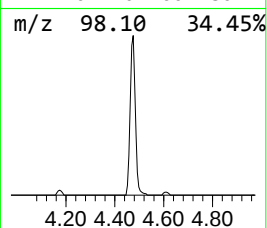
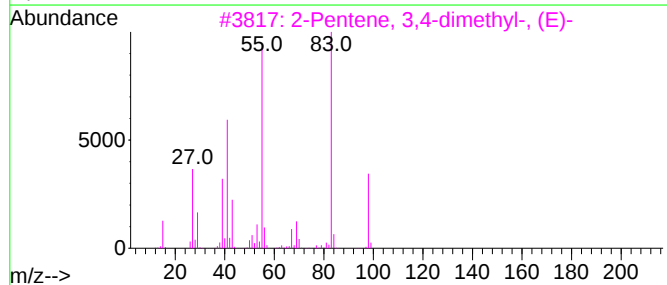
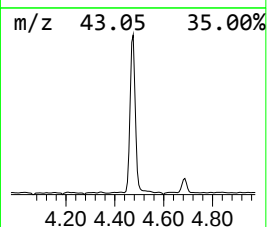
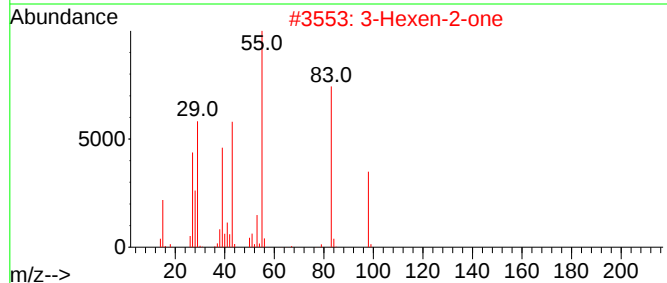
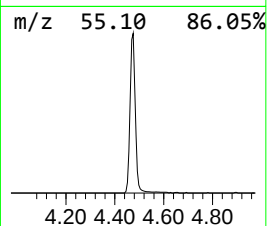
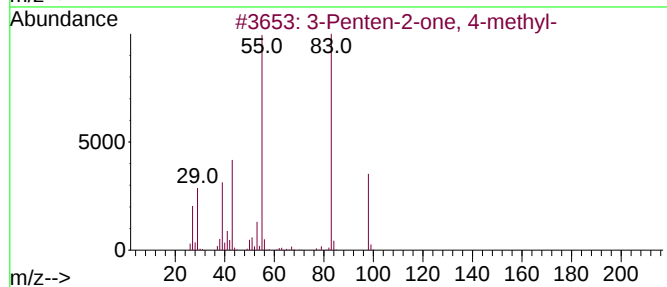
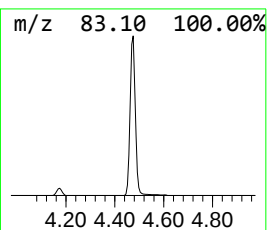
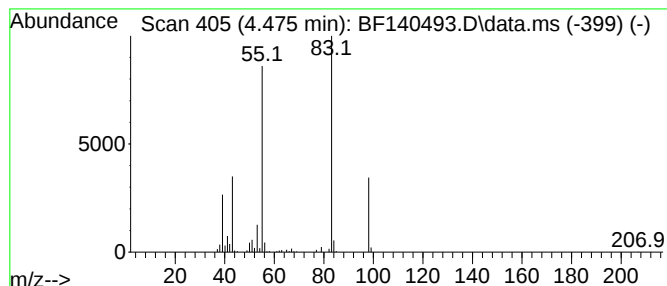
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.475	7.80 ng	264967	1,4-Dichlorobenzene-d4	6.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	94
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, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	86
5			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86



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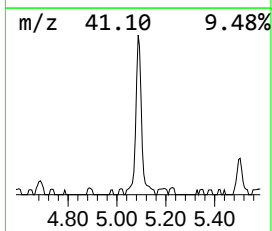
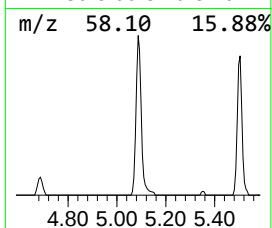
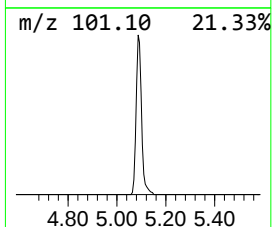
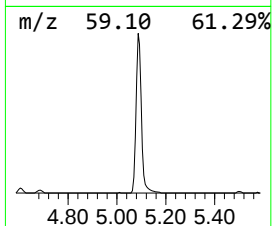
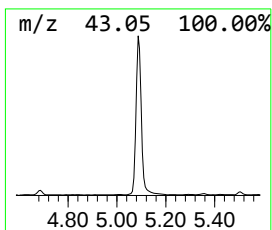
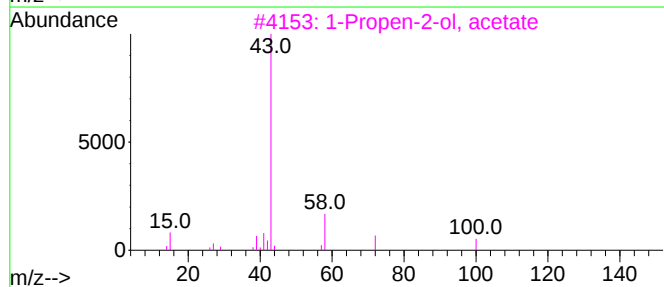
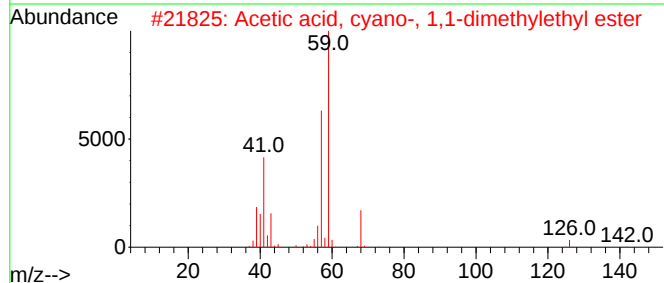
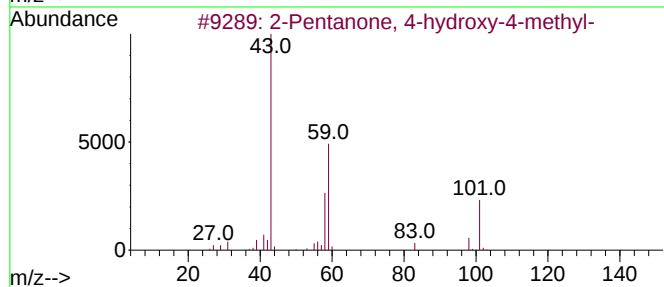
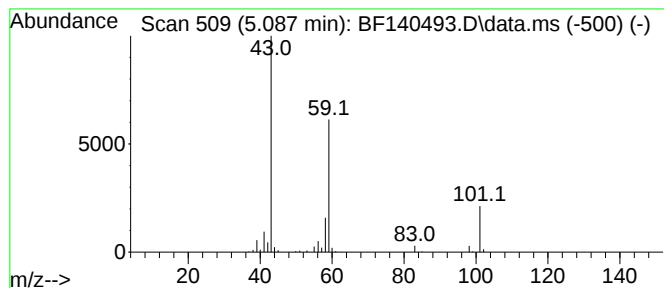
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.087	6.00 ng	203696	1,4-Dichlorobenzene-d4	6.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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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...	2.140	109.9	ng	3732740	1	6.875	679502	20.0
Trichloroethylene	2.522	181.1	ng	6152620	1	6.875	679502	20.0
3-Penten-2-one,...	4.475	7.8	ng	264967	1	6.875	679502	20.0
2-Pentanone, 4-...	5.087	6.0	ng	203696	1	6.875	679502	20.0