

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120622\
 Data File : BF131537.D
 Acq On : 06 Dec 2022 20:32
 Operator : CG\JU
 Sample : N5793-04
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 EB-2022-11-28

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-BF120522.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131537.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.222	16	23	29	rBV	1257231	1561232	37.14%	7.275%
2	4.522	410	414	419	rVB	51107	55549	1.32%	0.259%
3	5.146	513	520	528	rVB	672234	841081	20.01%	3.919%
4	5.534	581	586	589	rBV	1578520	1474766	35.08%	6.872%
5	5.928	650	653	657	rBV	109601	95103	2.26%	0.443%
6	6.540	752	757	760	rBV	1157352	1031316	24.53%	4.806%
7	6.922	818	822	825	rBV	666227	550716	13.10%	2.566%
8	7.492	912	919	922	rBV	1554876	1644015	39.11%	7.661%
9	8.210	1036	1041	1044	rBV	873711	711213	16.92%	3.314%
10	9.292	1219	1225	1228	rBV	4349746	3912737	93.08%	18.233%
11	9.975	1336	1341	1344	rBV	1133671	908396	21.61%	4.233%
12	10.769	1471	1476	1479	rBV	2759297	2345564	55.80%	10.930%
13	11.469	1591	1595	1598	rBV	1168172	954687	22.71%	4.449%
14	11.533	1602	1606	1609	rVB2	54818	43169	1.03%	0.201%
15	13.063	1861	1866	1869	rBV	4490806	4203599	100.00%	19.588%
16	14.121	2042	2046	2049	rBV	724636	618972	14.72%	2.884%
17	15.639	2297	2304	2314	rBV	378550	507889	12.08%	2.367%

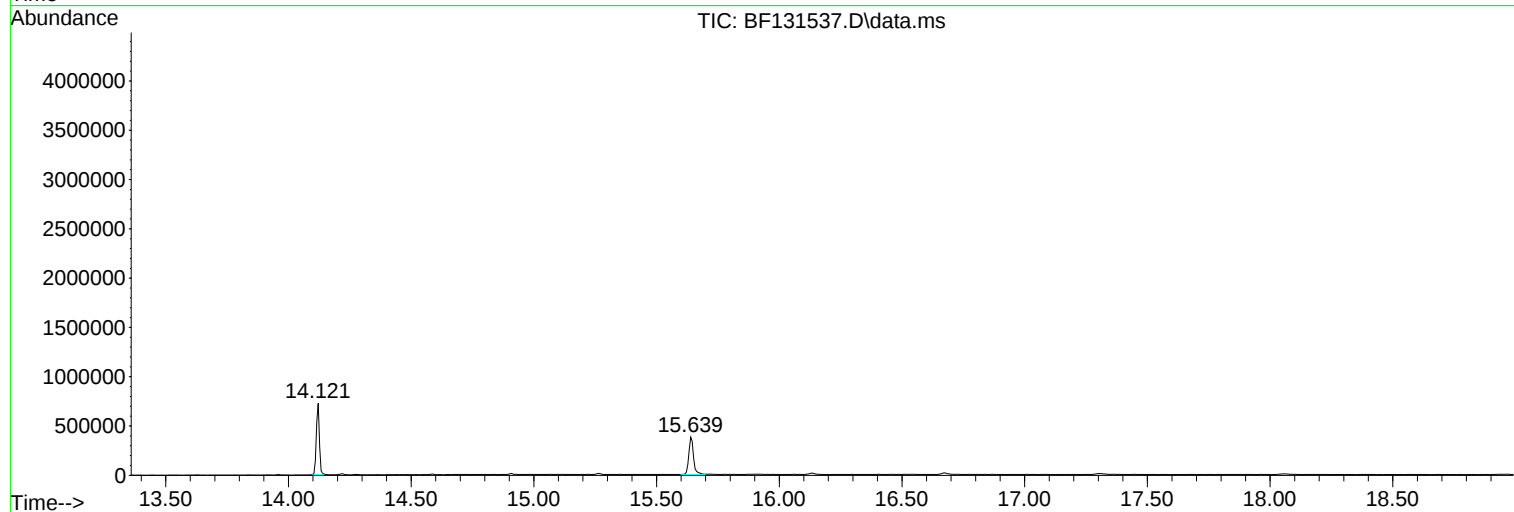
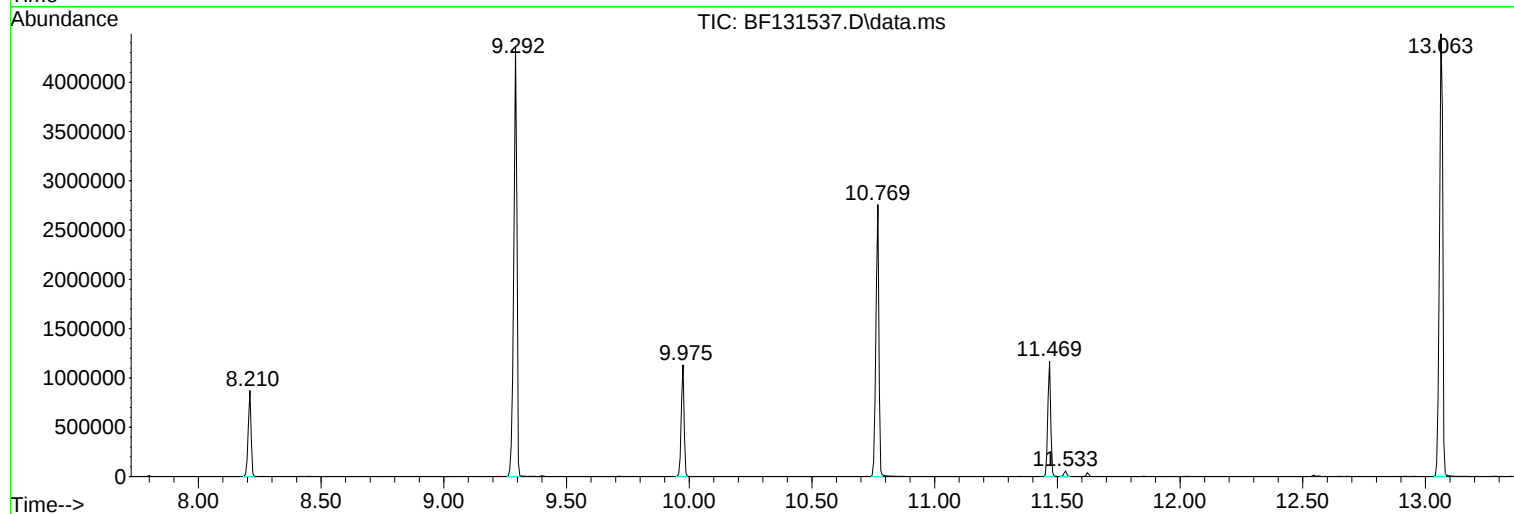
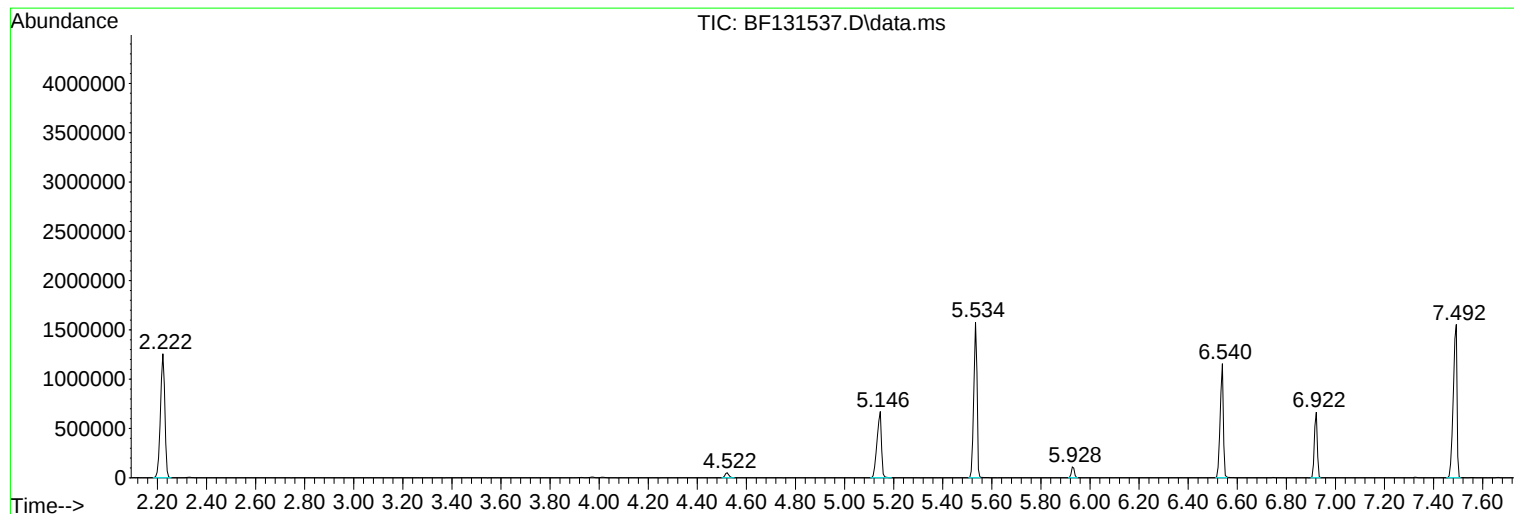
Sum of corrected areas: 21460004

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120522.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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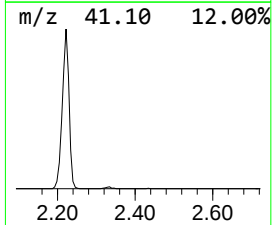
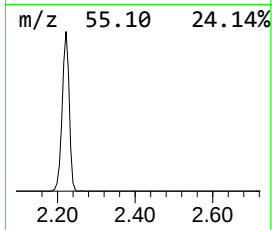
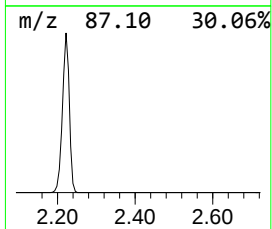
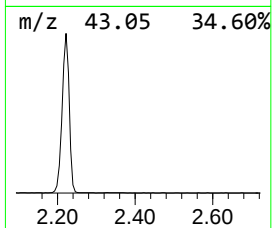
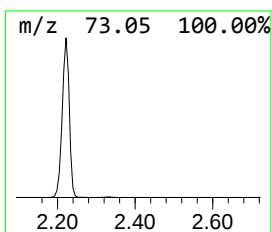
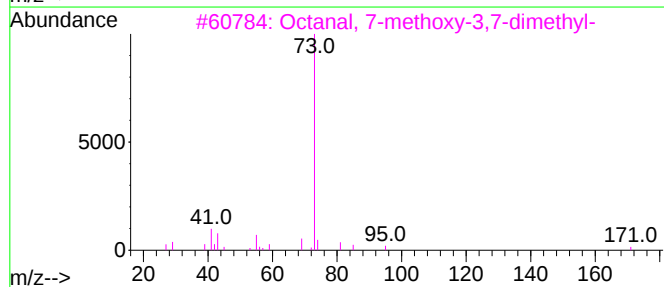
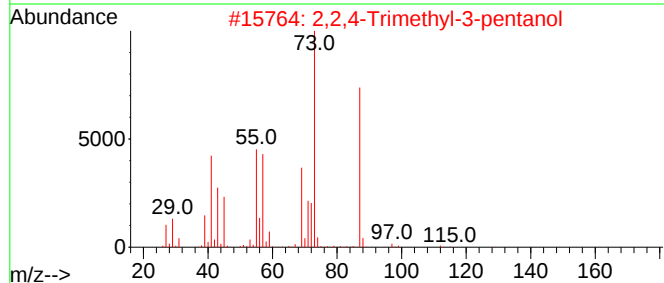
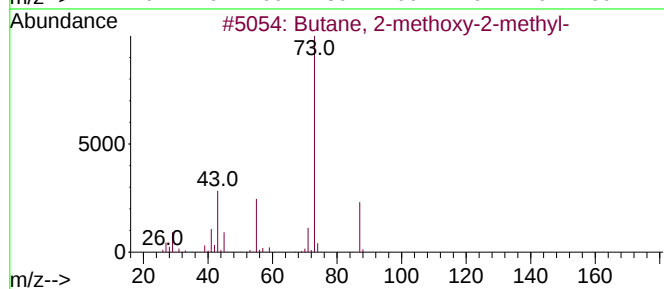
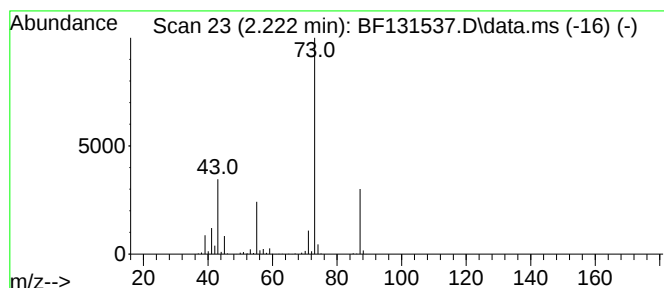
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.222	56.70 ng	1561230	1,4-Dichlorobenzene-d4	6.922

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	43
3			Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	23
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9



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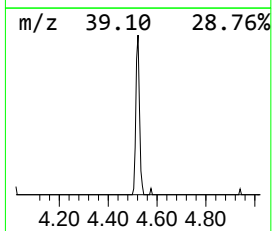
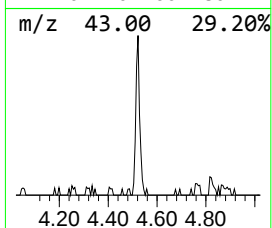
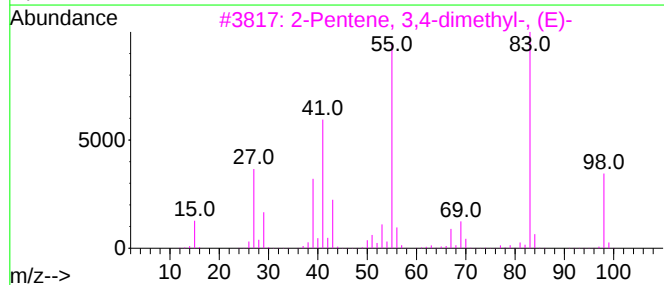
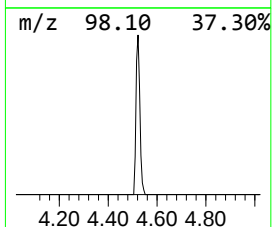
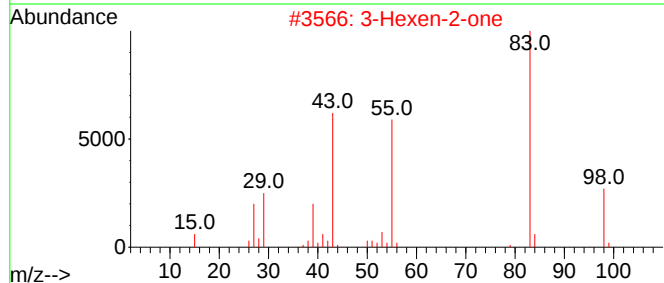
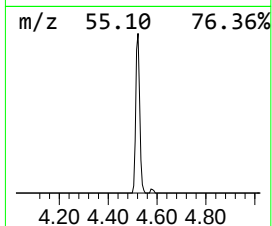
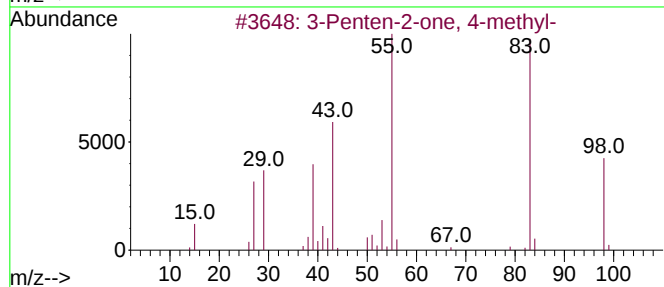
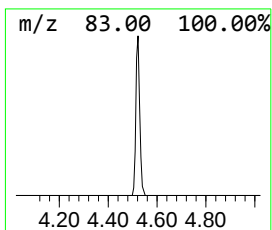
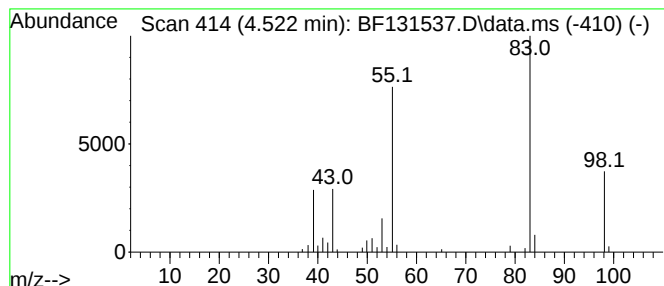
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.522	2.02 ng	55549	1,4-Dichlorobenzene-d4	6.922

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, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	90
5			2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	80



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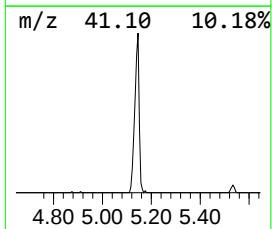
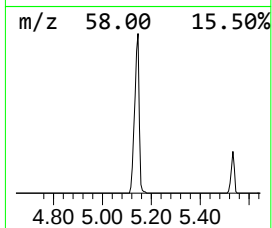
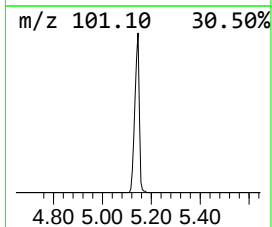
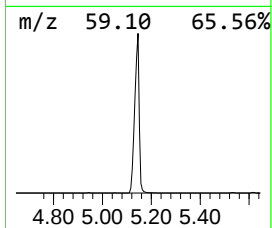
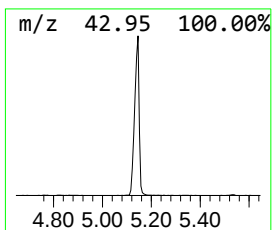
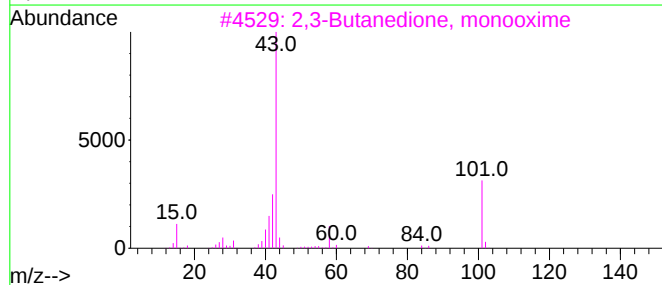
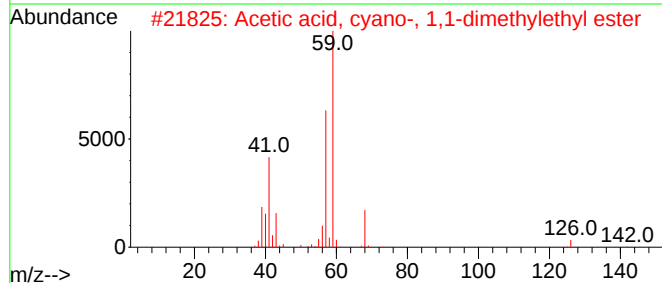
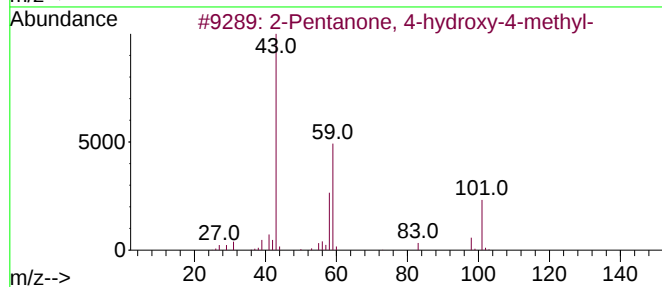
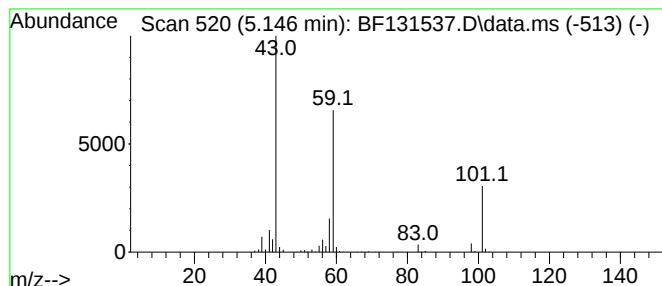
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.146	30.55 ng	841081	1,4-Dichlorobenzene-d4	6.922

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	25
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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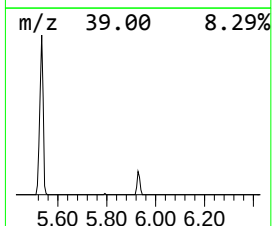
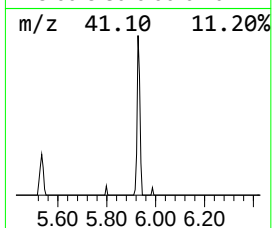
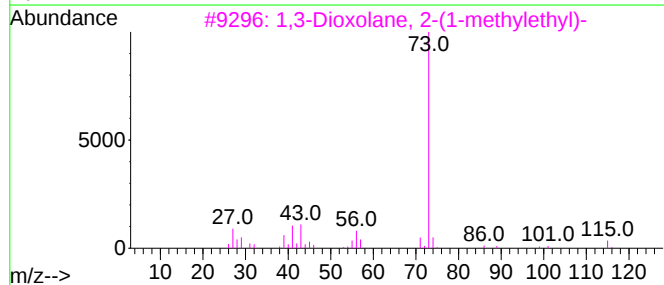
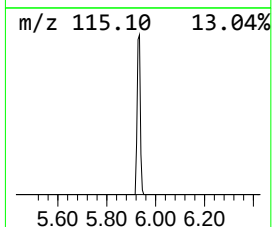
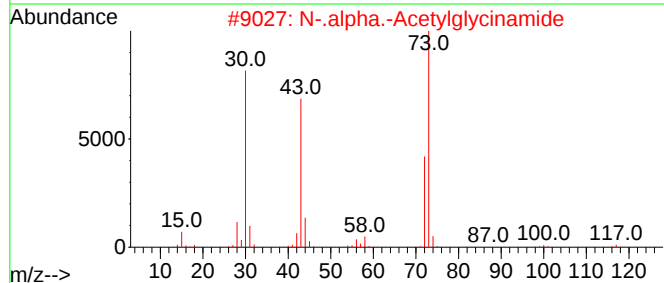
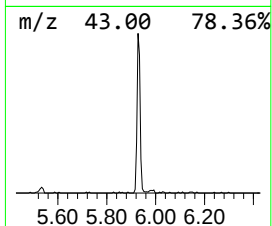
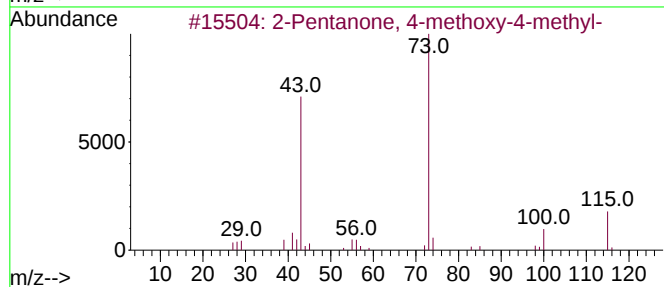
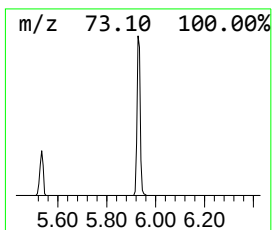
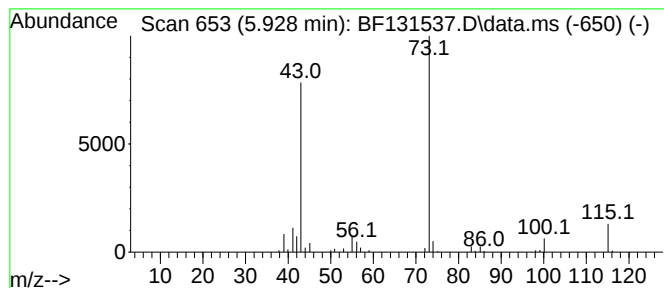
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Peak Number 4 2-Pentanone, 4-methoxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.928	3.45 ng	95103	1,4-Dichlorobenzene-d4	6.922

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	78
2			N-.alpha.-Acetylglycinamide	116	C4H8N2O2	002620-63-5	40
3			1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	32
4			Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	23
5			2-Pentanone, 3-ethyl-	114	C7H14O	006137-03-7	10



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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...	2.222	56.7	ng	1561230	1	6.922	550716	20.0
3-Penten-2-one,...	4.522	2.0	ng	55549	1	6.922	550716	20.0
2-Pentanone, 4-...	5.146	30.6	ng	841081	1	6.922	550716	20.0
2-Pentanone, 4-...	5.928	3.5	ng	95103	1	6.922	550716	20.0