

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121621\
 Data File : BF126212.D
 Acq On : 16 Dec 2021 15:20
 Operator : JU/CG
 Sample : M5022-39
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP13

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-BF121521.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126212.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.205	15	20	26	rVB	80772	106166	2.37%	0.305%
2	4.399	388	393	397	rBV	116048	128873	2.88%	0.371%
3	5.028	493	500	503	rBV	2421184	2994608	66.85%	8.609%
4	5.428	562	568	571	rBV	4219882	4130194	92.20%	11.874%
5	5.828	633	636	640	rVB	147129	119407	2.67%	0.343%
6	6.434	734	739	743	rBV	3935966	4479371	100.00%	12.878%
7	6.816	800	804	807	rBV	1361238	1142445	25.50%	3.285%
8	7.375	894	899	902	rBV	3189305	2936462	65.56%	8.442%
9	7.998	1000	1005	1008	rBV	91605	72831	1.63%	0.209%
10	8.098	1017	1022	1025	rBV	1671164	1580498	35.28%	4.544%
11	9.175	1200	1205	1208	rBV	4867360	4467435	99.73%	12.844%
12	9.263	1216	1220	1224	rBV2	77823	67006	1.50%	0.193%
13	9.657	1282	1287	1294	rBV3	79242	86258	1.93%	0.248%
14	9.851	1316	1320	1323	rBV	1995635	1671830	37.32%	4.807%
15	10.263	1386	1390	1393	rBV2	50532	53277	1.19%	0.153%
16	10.633	1449	1453	1456	rBV	2617171	2381989	53.18%	6.848%
17	11.210	1544	1551	1554	rBV5	45944	71745	1.60%	0.206%
18	11.304	1563	1567	1568	rBV	61880	54401	1.21%	0.156%
19	11.333	1568	1572	1575	rVV	2011354	1626231	36.30%	4.675%
20	11.504	1596	1601	1604	rBV	50531	58430	1.30%	0.168%
21	11.898	1666	1668	1672	rVB	105254	88559	1.98%	0.255%
22	12.322	1736	1740	1743	rBV	51204	50496	1.13%	0.145%
23	12.380	1747	1750	1754	rVB	59779	56983	1.27%	0.164%
24	12.922	1837	1842	1845	rBV	4100512	3910102	87.29%	11.242%
25	13.457	1928	1933	1939	rBV	45797	55063	1.23%	0.158%
26	13.580	1951	1954	1957	rVB	54156	51223	1.14%	0.147%
27	13.821	1991	1995	2002	rBV	248938	263911	5.89%	0.759%
28	13.892	2004	2007	2011	rVB	56412	52336	1.17%	0.150%
29	13.963	2016	2019	2023	rVV	1028376	976599	21.80%	2.808%
30	15.410	2260	2265	2272	rBV2	906935	1047922	23.39%	3.013%

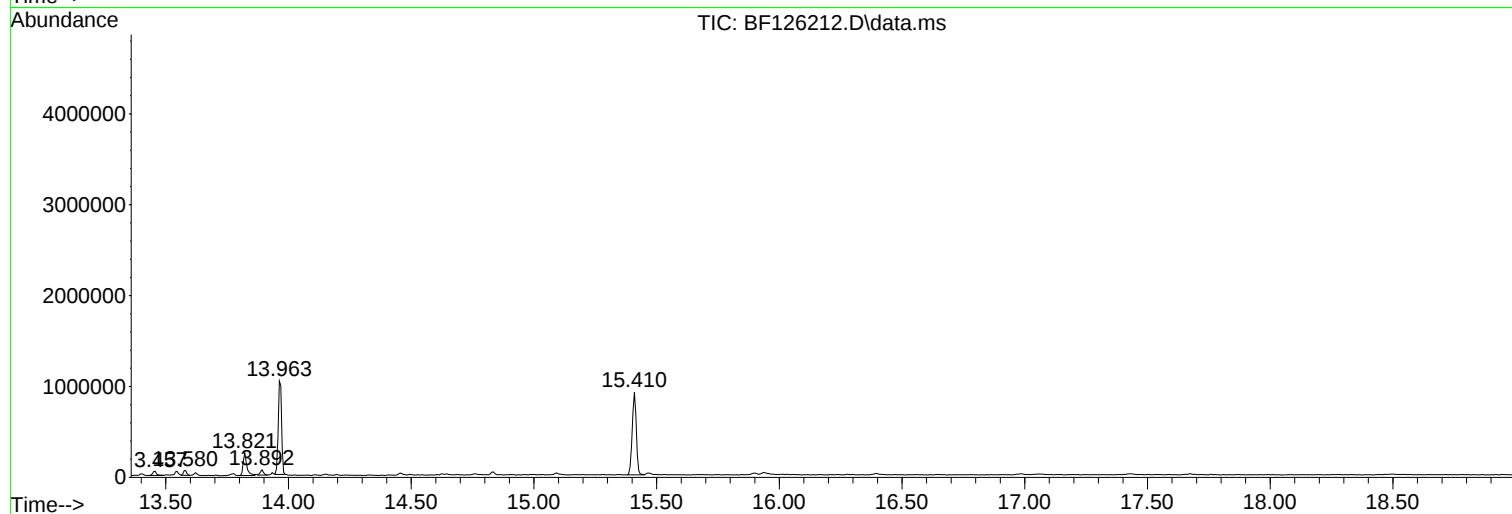
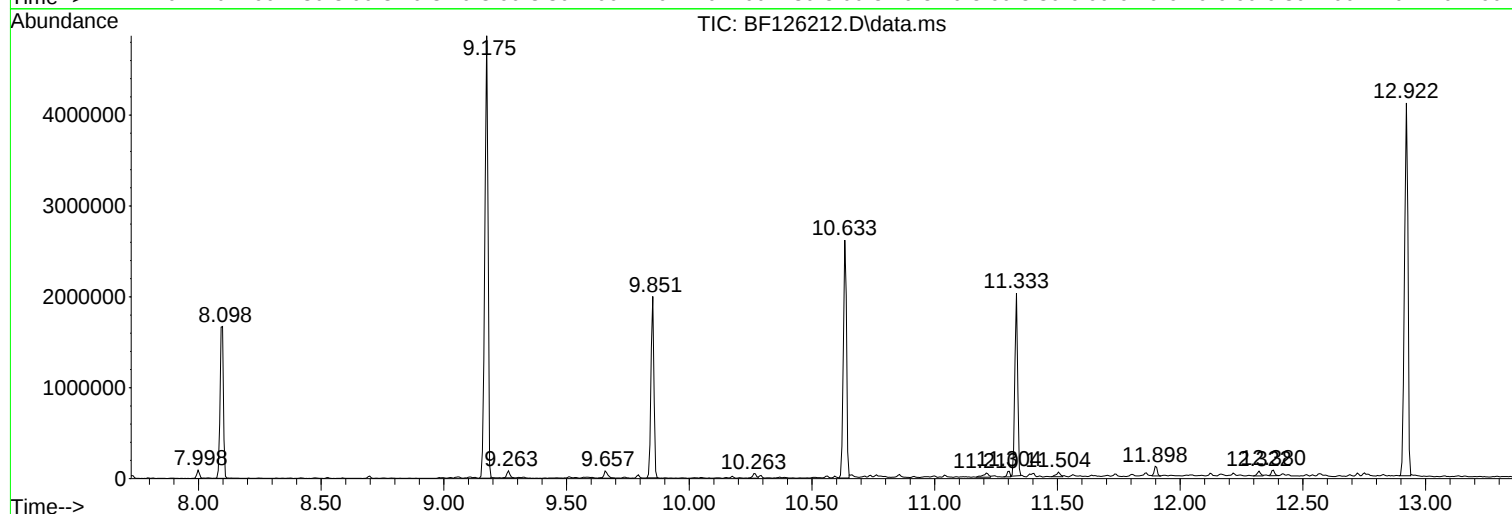
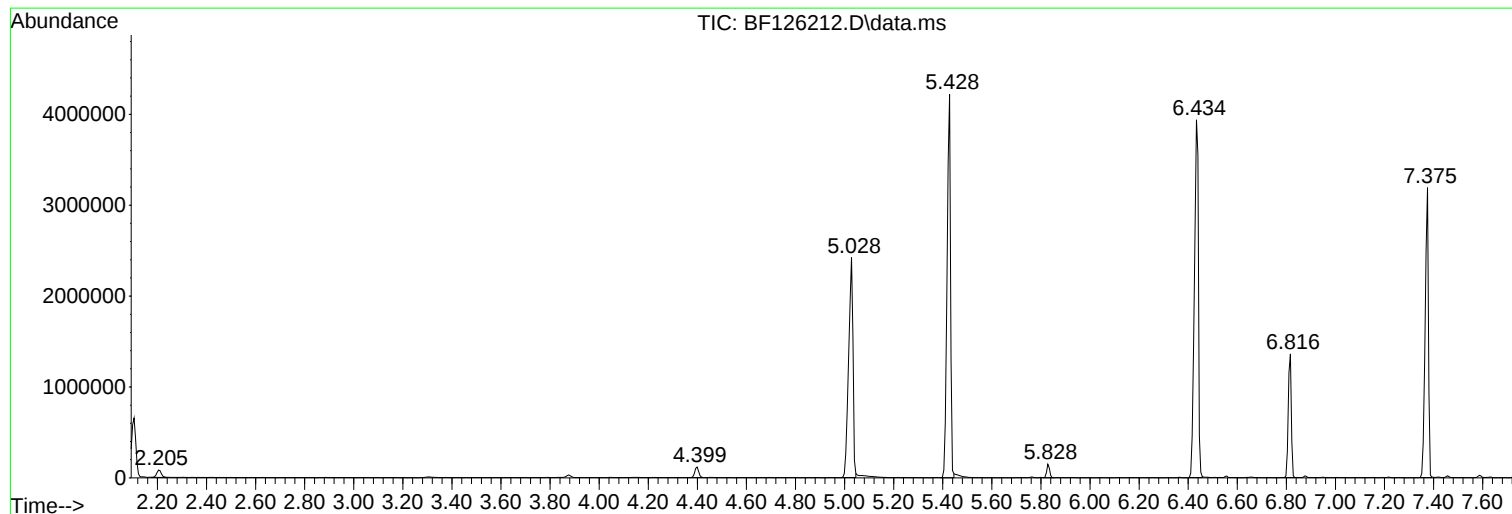
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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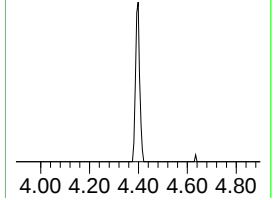
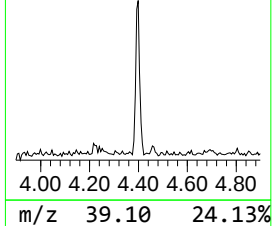
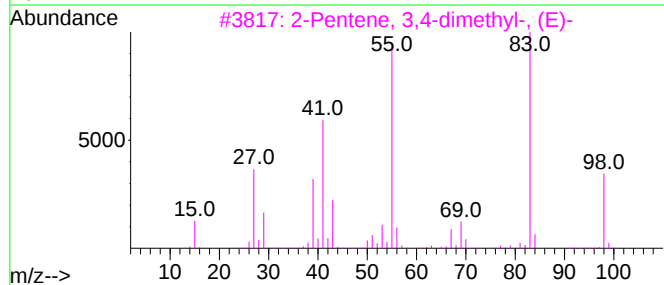
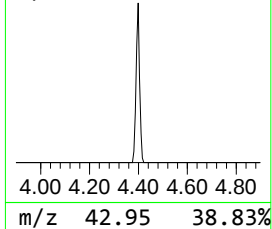
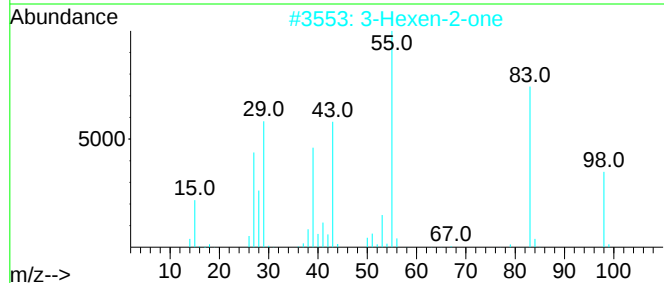
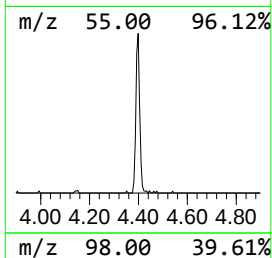
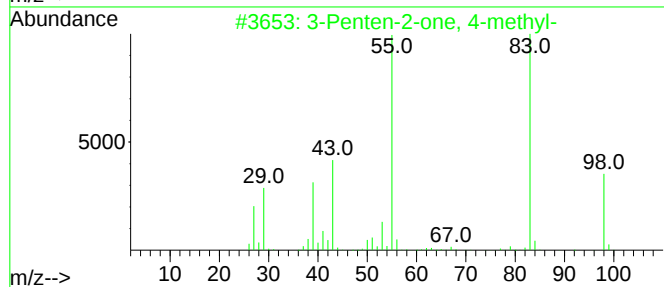
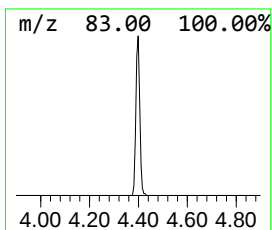
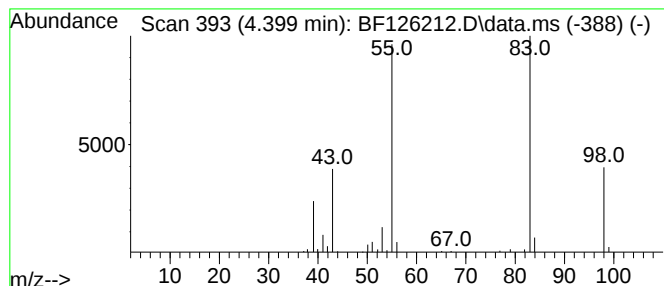
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.399	2.26 ng	128873	1,4-Dichlorobenzene-d4	6.816

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	86
5			2,4-Azetidinedione, 3,3-diethyl-	141	C7H11NO2	042282-85-9	83



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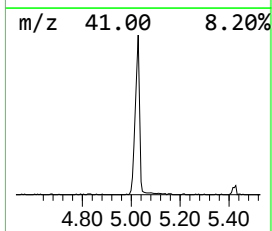
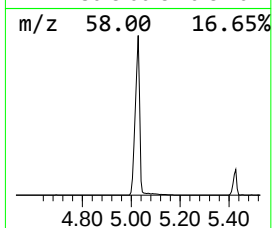
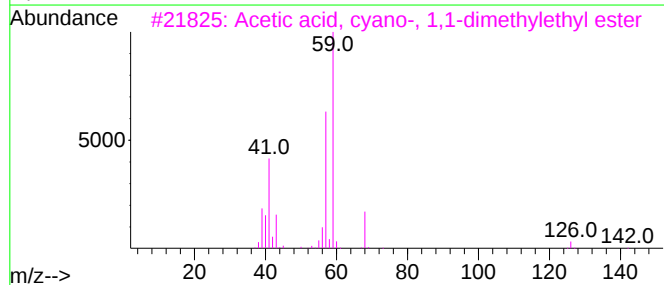
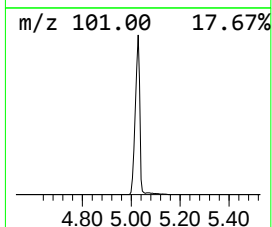
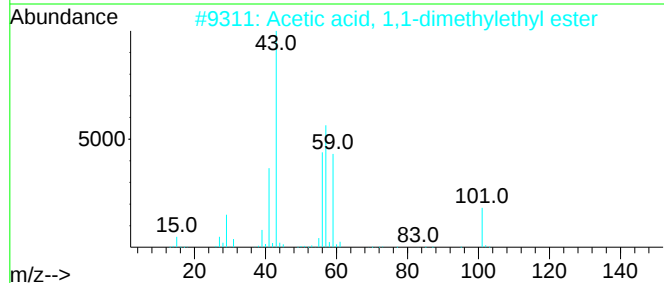
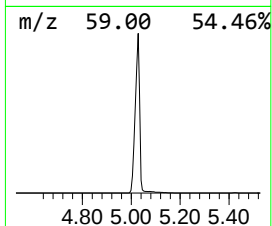
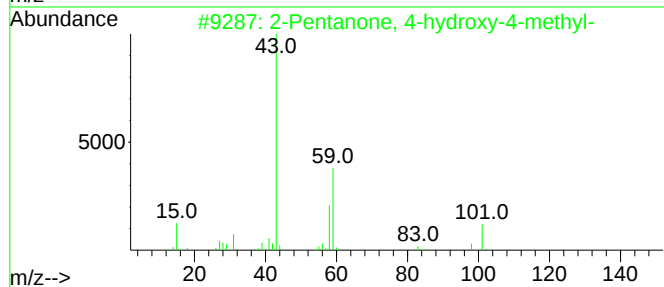
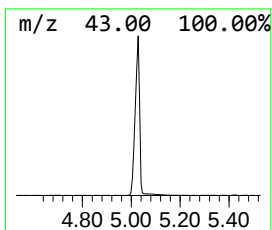
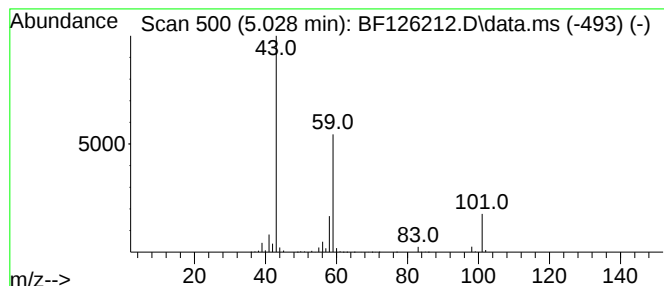
Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.028	52.42 ng	2994610	1,4-Dichlorobenzene-d4	6.816	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	Acetone	58	C3H6O	000067-64-1	9
5	Ethanol, pentamethyl-	116	C7H16O	000594-83-2	9



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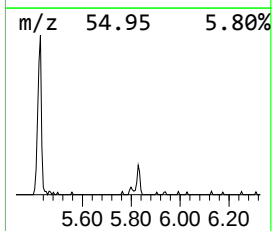
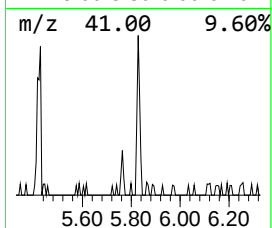
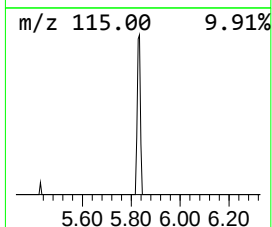
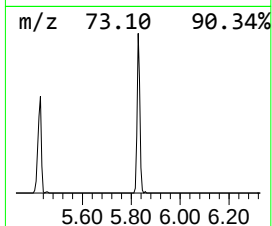
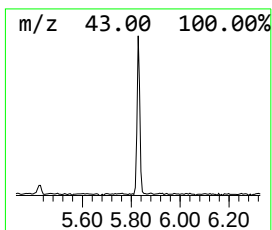
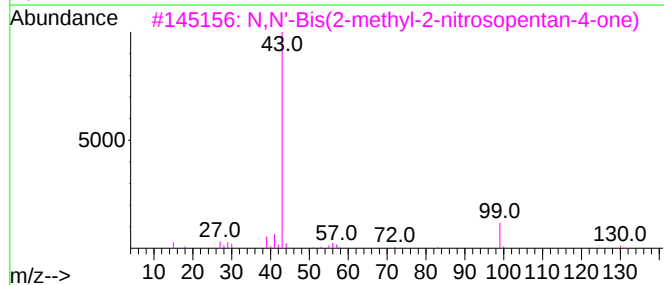
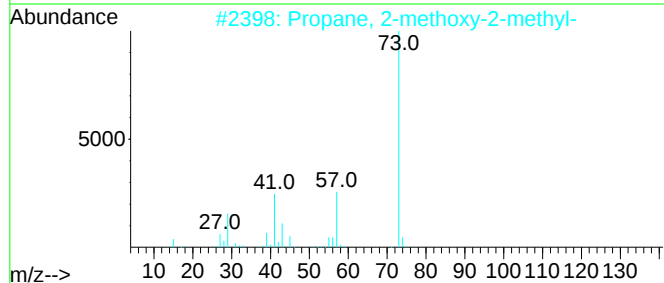
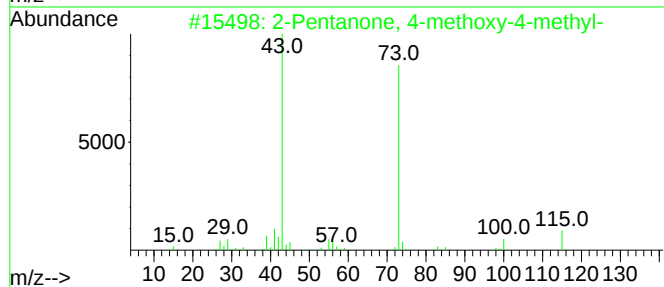
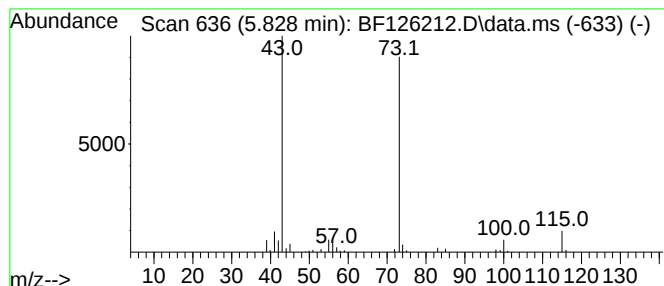
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.828	2.09 ng	119407	1,4-Dichlorobenzene-d4	6.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2			Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	12
3			N,N'-Bis(2-methyl-2-nitrosopenta...	258	C12H22N2O4	094514-30-4	10
4			Morpholine, 2,6-dimethyl-	115	C6H13NO	000141-91-3	9
5			2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	9



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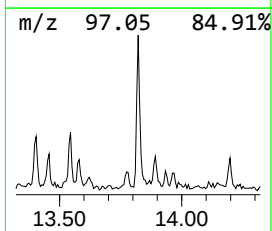
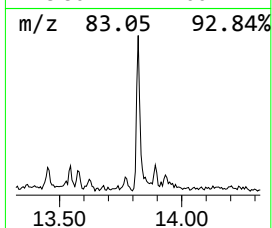
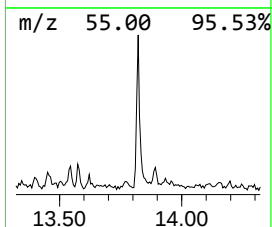
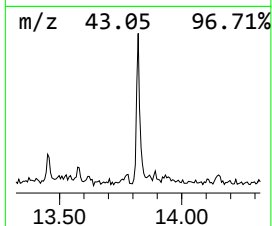
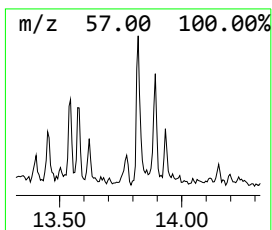
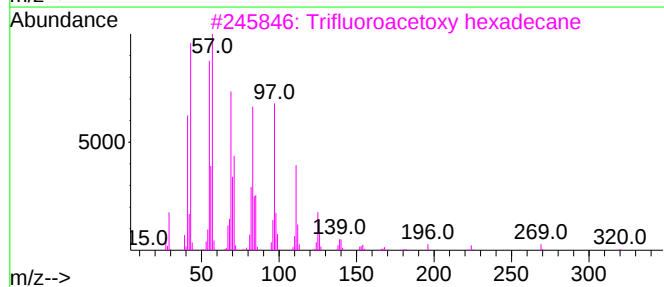
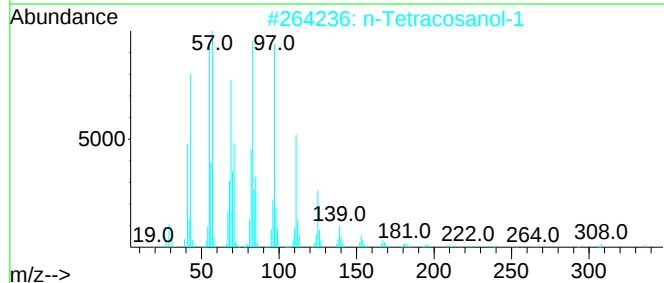
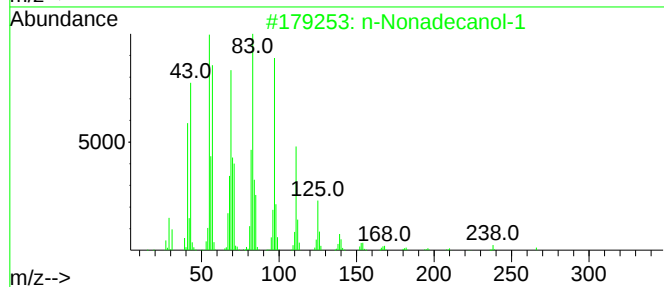
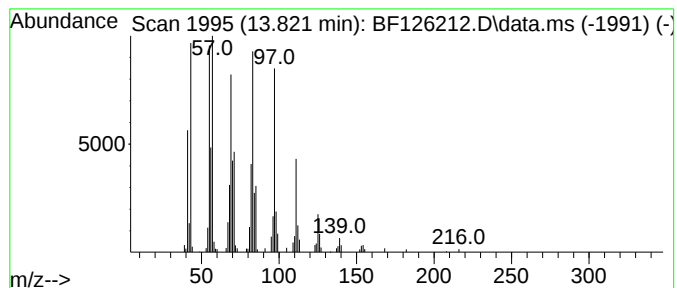
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 n-Nonadecanol-1 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.822	5.40 ng	263911	Chrysene-d12	13.969

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Nonadecanol-1	284	C19H40O	001454-84-8	94
2			n-Tetracosanol-1	354	C24H50O	000506-51-4	94
3			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
4			Behenic alcohol	326	C22H46O	000661-19-8	93
5			1-Hexacosanol	382	C26H54O	000506-52-5	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one,...	4.399	2.3	ng	128873	1	6.816	1142450	20.0
2-Pentanone, 4-...	5.028	52.4	ng	2994610	1	6.816	1142450	20.0
2-Pentanone, 4-...	5.828	2.1	ng	119407	1	6.816	1142450	20.0
n-Nonadecanol-1	13.822	5.4	ng	263911	5	13.969	976599	20.0