

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022322\
 Data File : BF127037.D
 Acq On : 23 Feb 2022 14:06
 Operator : CG\JU
 Sample : N1626-15
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CC-A8

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-BF021622.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF127037.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.699	232	240	247	rBV	593506	919708	2.47%	1.564%
2	4.634	376	399	402	rBV	9141591	37266116	100.00%	63.359%
3	5.198	480	495	498	rBV	3629366	9618556	25.81%	16.353%
4	6.904	782	785	789	rBV	601682	497593	1.34%	0.846%
5	7.228	835	840	843	rBV	1151806	1114082	2.99%	1.894%
6	7.469	876	881	884	rBV	1700385	1557942	4.18%	2.649%
7	8.186	999	1003	1009	rVB	757631	692297	1.86%	1.177%
8	9.263	1180	1186	1189	rBV	3203698	2820525	7.57%	4.795%
9	9.945	1295	1302	1306	rBV	951937	751854	2.02%	1.278%
10	11.433	1552	1555	1559	rBV	834531	737301	1.98%	1.254%
11	13.027	1821	1826	1829	rVB	2617720	2437440	6.54%	4.144%
12	14.833	2129	2133	2140	rBV	404516	403637	1.08%	0.686%

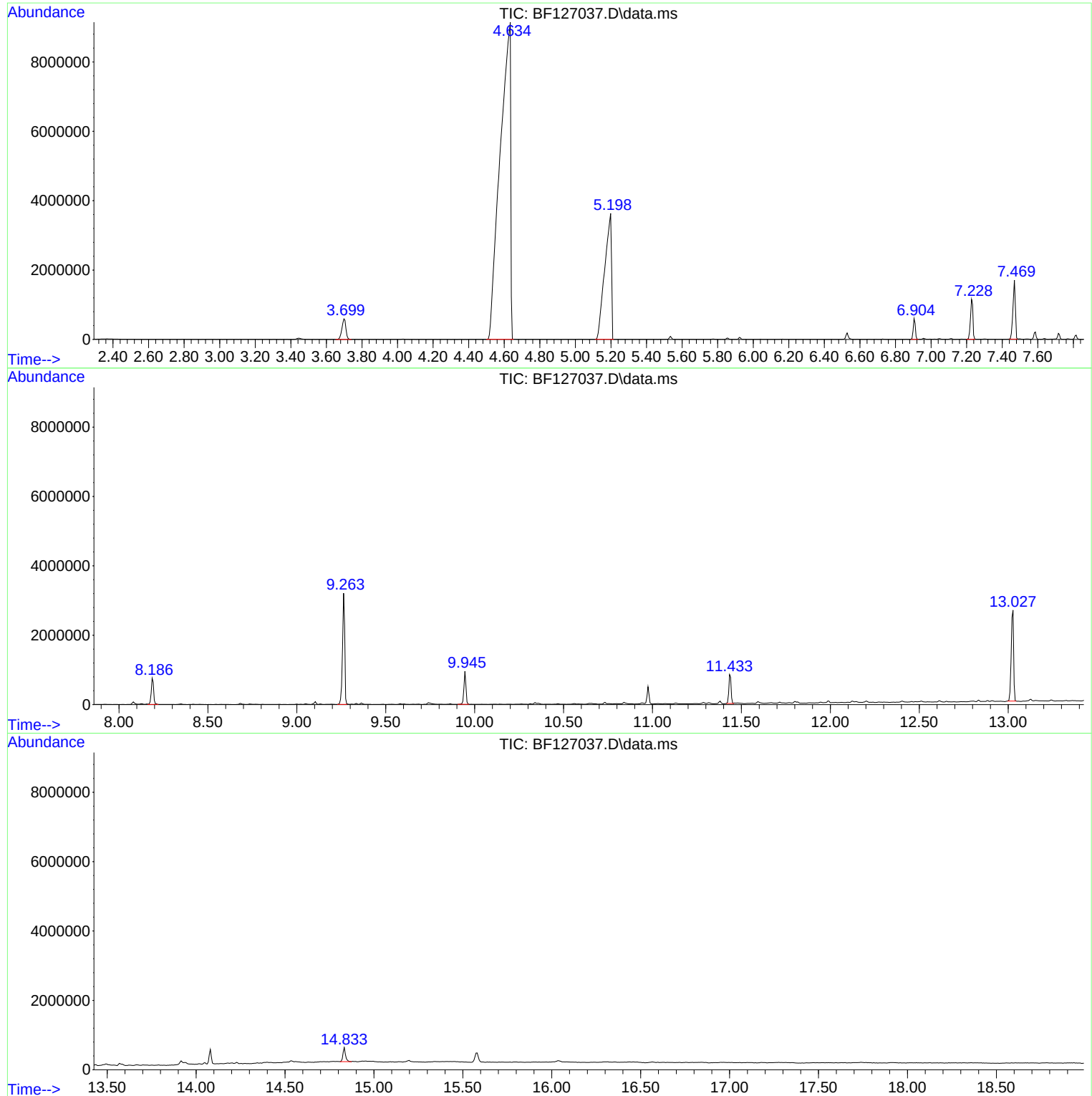
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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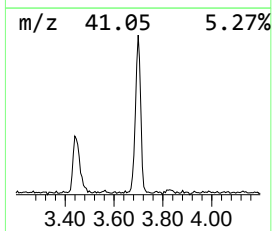
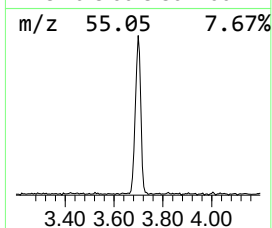
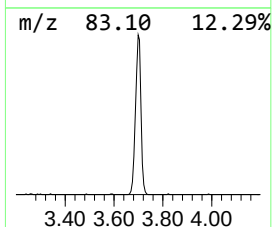
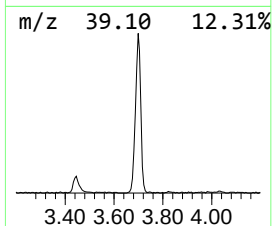
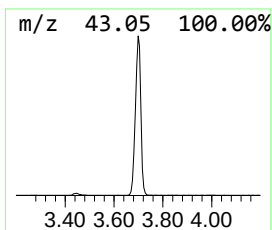
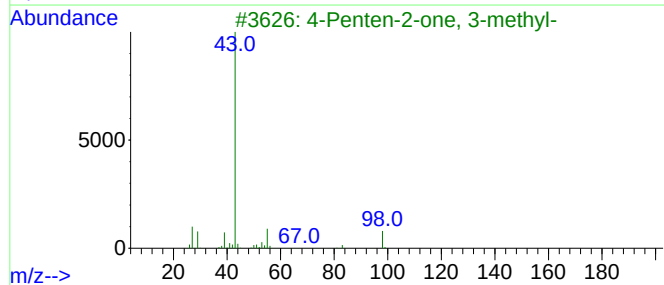
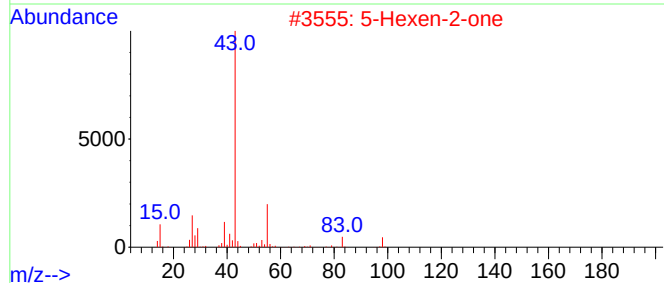
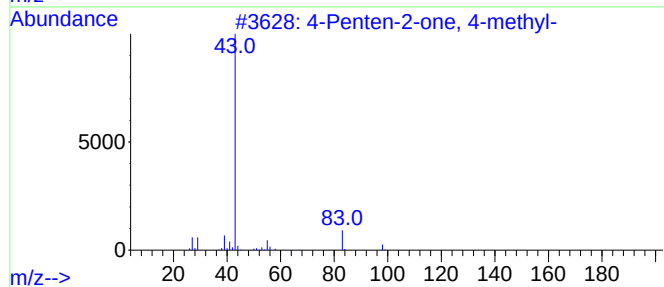
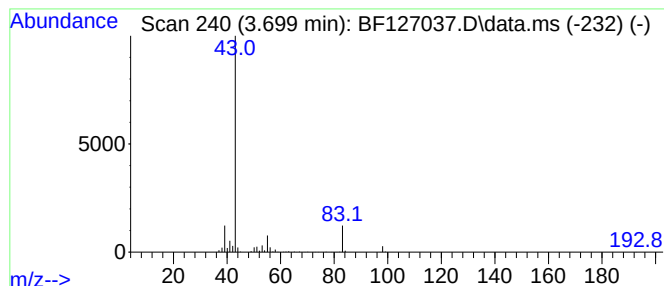
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.699	36.97 ng	919708	1,4-Dichlorobenzene-d4	6.904

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	86
2		5-Hexen-2-one	98	C6H10O	000109-49-9	50
3		4-Penten-2-one, 3-methyl-	98	C6H10O	000758-87-2	47
4		2-Pentanone, 3-methylene-	98	C6H10O	004359-77-7	17
5		Methyl 1-methylcyclopropyl ketone	98	C6H10O	001567-75-5	12



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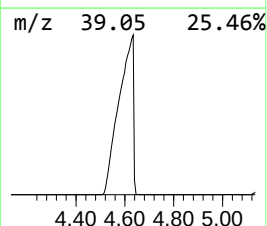
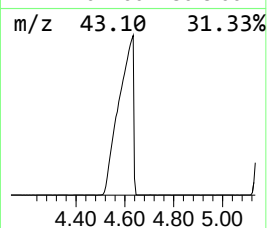
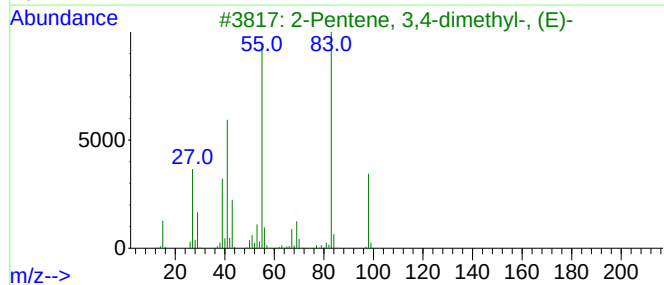
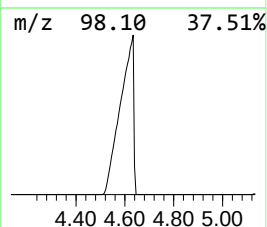
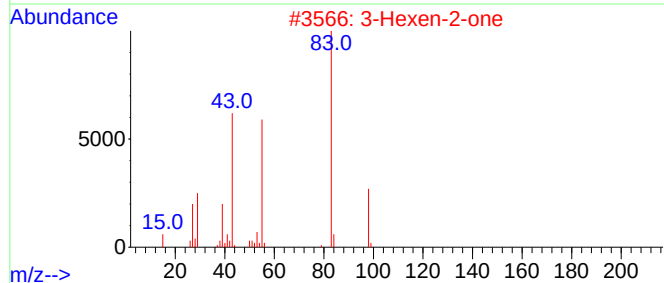
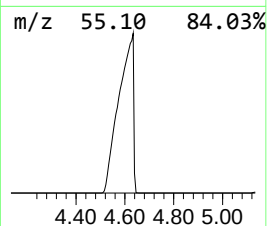
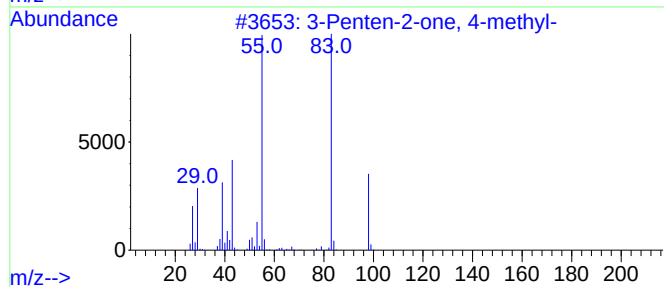
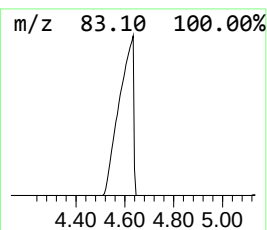
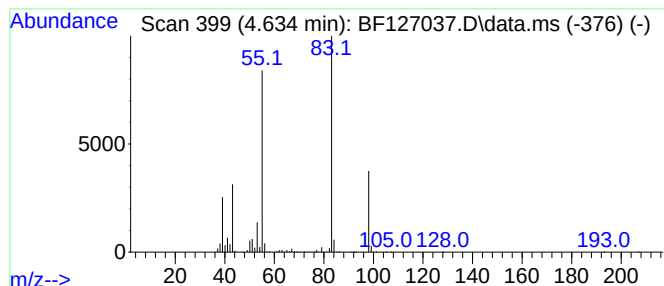
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.634	1497.86 ng	37266100	1,4-Dichlorobenzene-d4	6.904

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	95
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			Furan, 2-methoxy-	98	C5H6O2	025414-22-6	78



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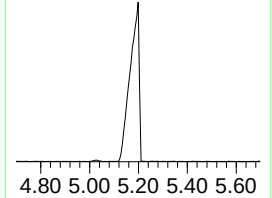
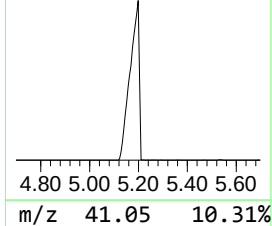
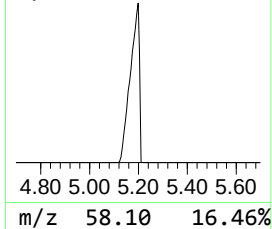
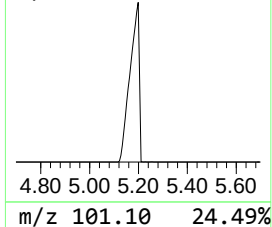
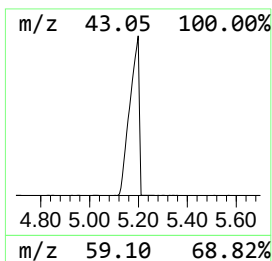
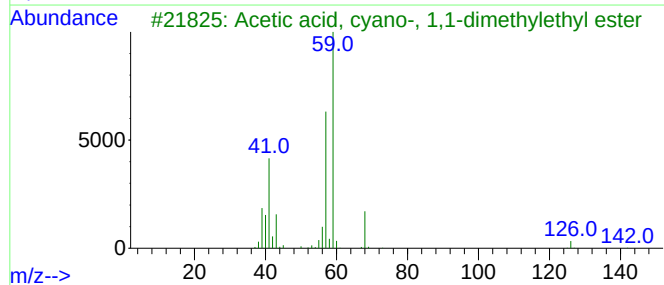
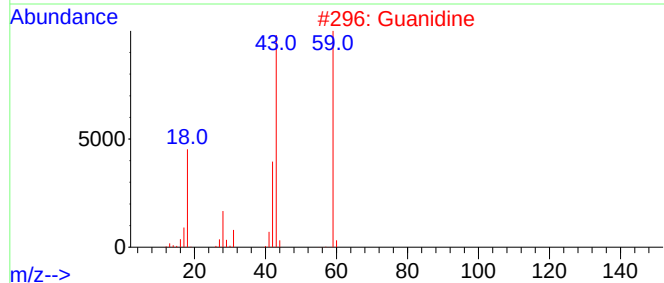
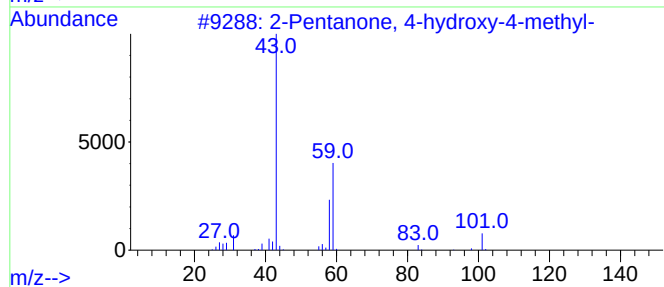
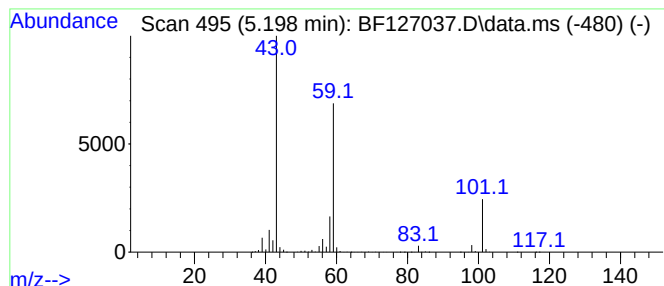
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.198	386.60 ng	9618560	1,4-Dichlorobenzene-d4	6.904	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Guanidine	59	CH5N3	000113-00-8	43
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
5	Acetone	58	C3H6O	000067-64-1	10



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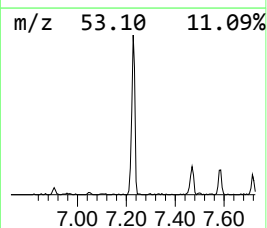
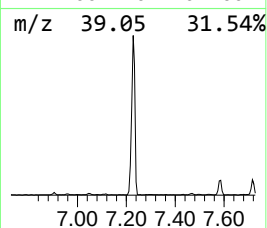
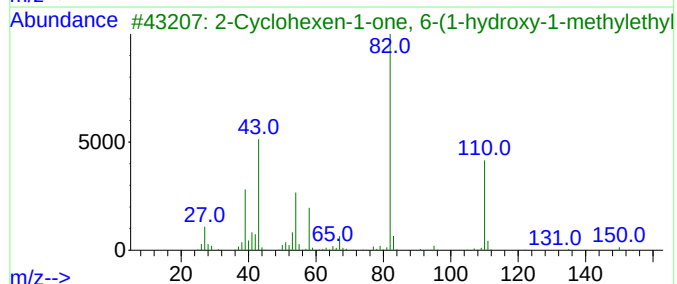
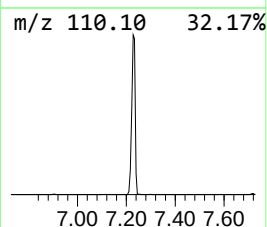
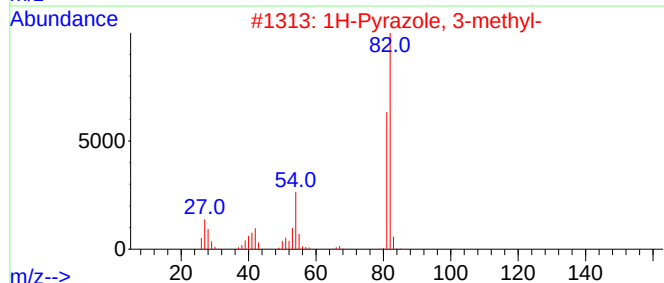
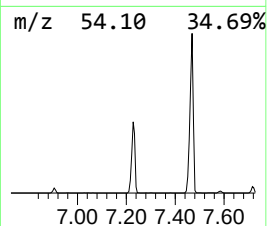
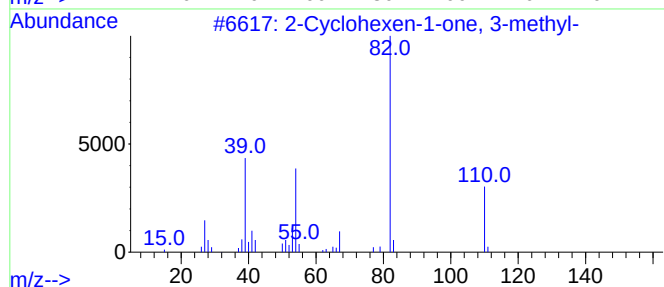
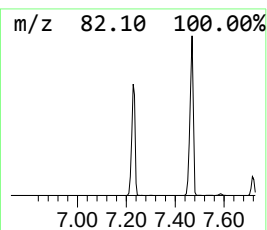
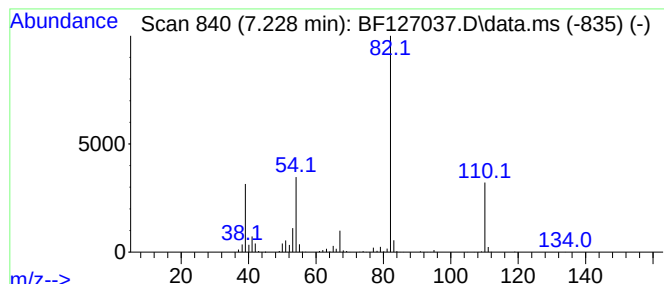
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Peak Number 4 2-Cyclohexen-1-one, 3-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.228	44.78 ng	1114080	1,4-Dichlorobenzene-d4	6.904

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Cyclohexen-1-one, 3-methyl-	110	C7H10O	001193-18-6	91
2			1H-Pyrazole, 3-methyl-	82	C4H6N2	001453-58-3	59
3			2-Cyclohexen-1-one, 6-(1-hydroxy...	168	C10H16O2	087791-00-2	56
4			2-Cyclopenten-1-one	82	C5H6O	000930-30-3	50
5			Betazole	111	C5H9N3	000105-20-4	40



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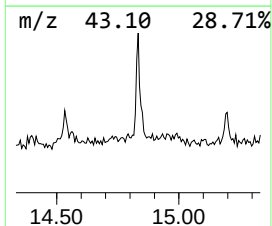
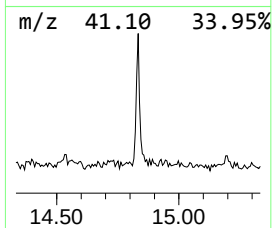
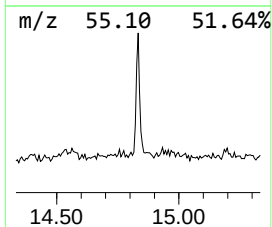
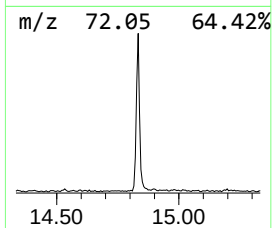
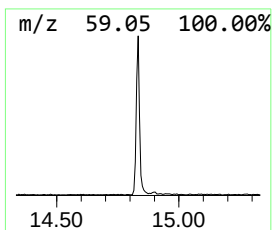
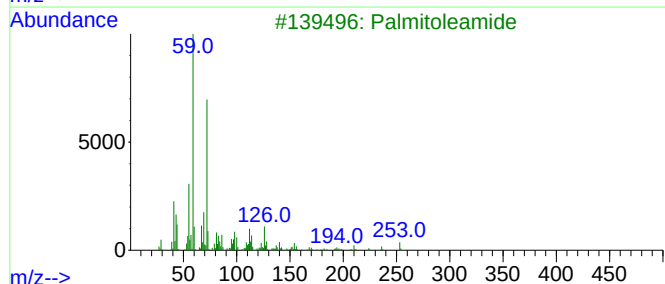
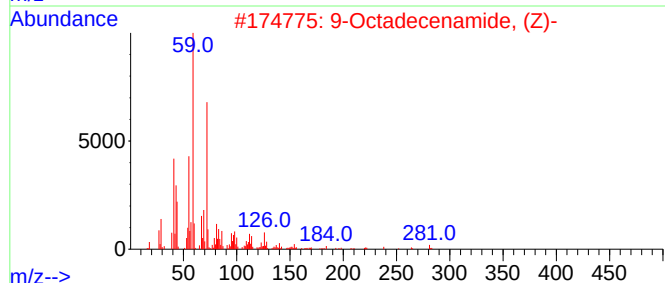
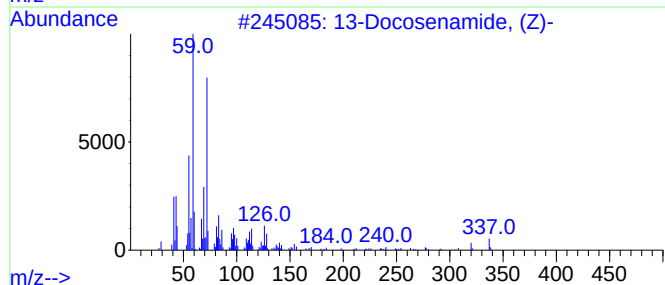
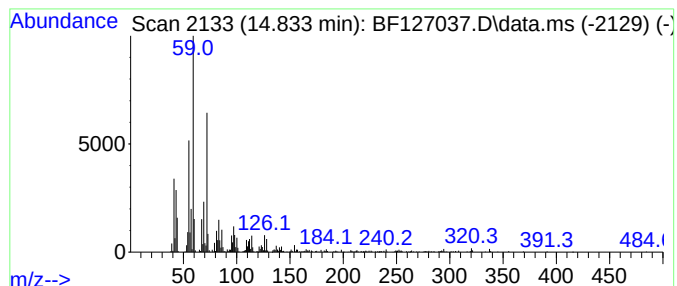
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Peak Number 5 13-Docosenamide, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.833	20.00 ng	403637	Perylene-d12	15.580

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	93
2			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	87
3			Palmitoleamide	253	C16H31NO	106010-22-4	81
4			Tetradecanamide	227	C14H29NO	000638-58-4	72
5			Octanamide	143	C8H17NO	000629-01-6	59



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
4-Penten-2-one,...	3.699	37.0	ng	919708	1	6.904	497593	20.0
3-Penten-2-one,...	4.634	1497.9	ng	37266100	1	6.904	497593	20.0
2-Pentanone, 4-...	5.198	386.6	ng	9618560	1	6.904	497593	20.0
2-Cyclohexen-1-...	7.228	44.8	ng	1114080	1	6.904	497593	20.0
13-Docosenamide...	14.833	20.0	ng	403637	6	15.580	403637	20.0