

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121120\
 Data File : BF122665.D
 Acq On : 11 Dec 2020 16:09
 Operator : JU/CG
 Sample : L5014-01
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 351

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-BF120520.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF122665.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.551	243	249	259	rBV	238907	376829	2.66%	1.113%
2	4.475	393	406	409	rBV	5754239	14176939	100.00%	41.859%
3	5.063	499	506	509	rBV	1912752	2591598	18.28%	7.652%
4	6.463	740	744	760	rBV	454976	495132	3.49%	1.462%
5	6.839	804	808	811	rBV	1004078	795895	5.61%	2.350%
6	7.157	859	862	874	rBV	252631	215498	1.52%	0.636%
7	7.398	899	903	915	rBV	1806135	1738234	12.26%	5.132%
8	7.651	943	946	955	rVB	160273	152136	1.07%	0.449%
9	8.122	1022	1026	1041	rBV	1148903	1056863	7.45%	3.121%
10	9.198	1204	1209	1220	rBV	3677685	3409701	24.05%	10.068%
11	9.874	1320	1324	1340	rVB	1210691	1230835	8.68%	3.634%
12	11.363	1573	1577	1582	rBV	1332514	1261157	8.90%	3.724%
13	12.951	1842	1847	1850	rBV	3836174	3787581	26.72%	11.183%
14	14.004	2022	2026	2034	rVB	1160057	1195455	8.43%	3.530%
15	14.851	2166	2170	2176	rVB	314466	329137	2.32%	0.972%
16	15.462	2269	2274	2291	rBV	683962	1055308	7.44%	3.116%

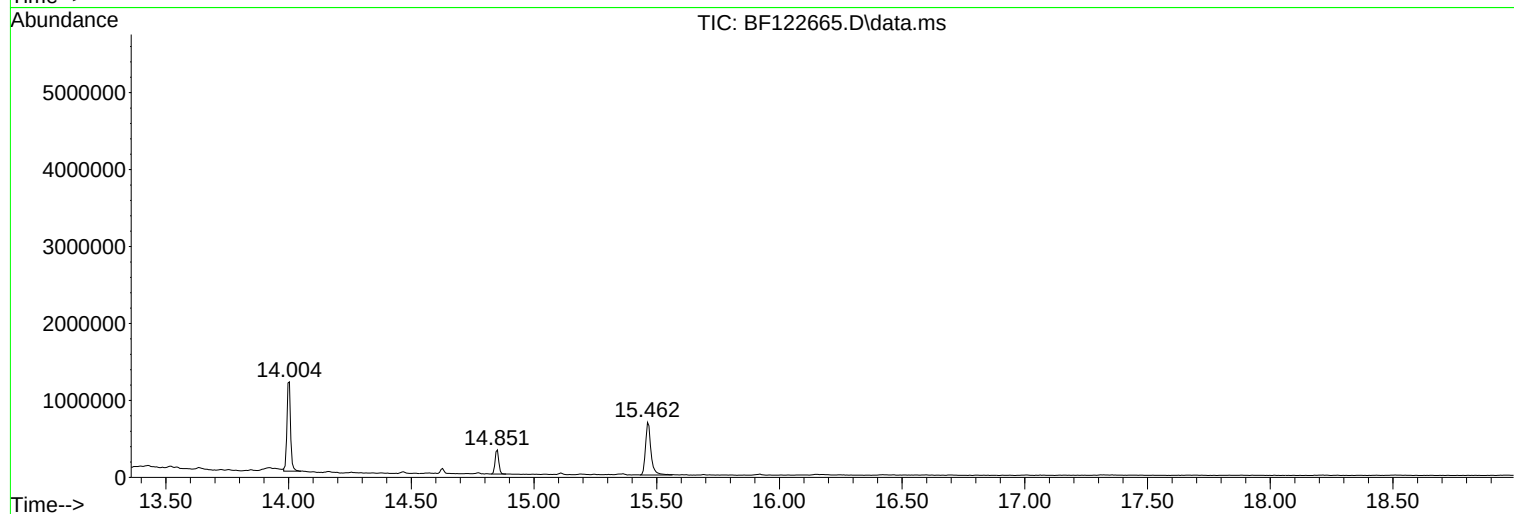
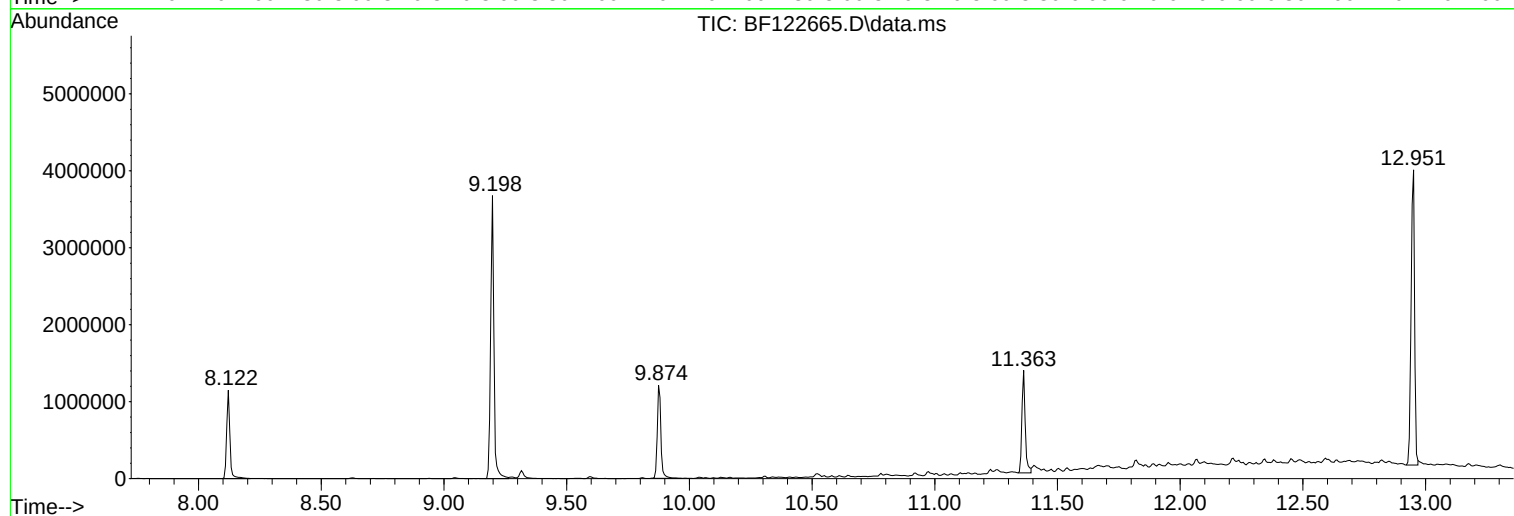
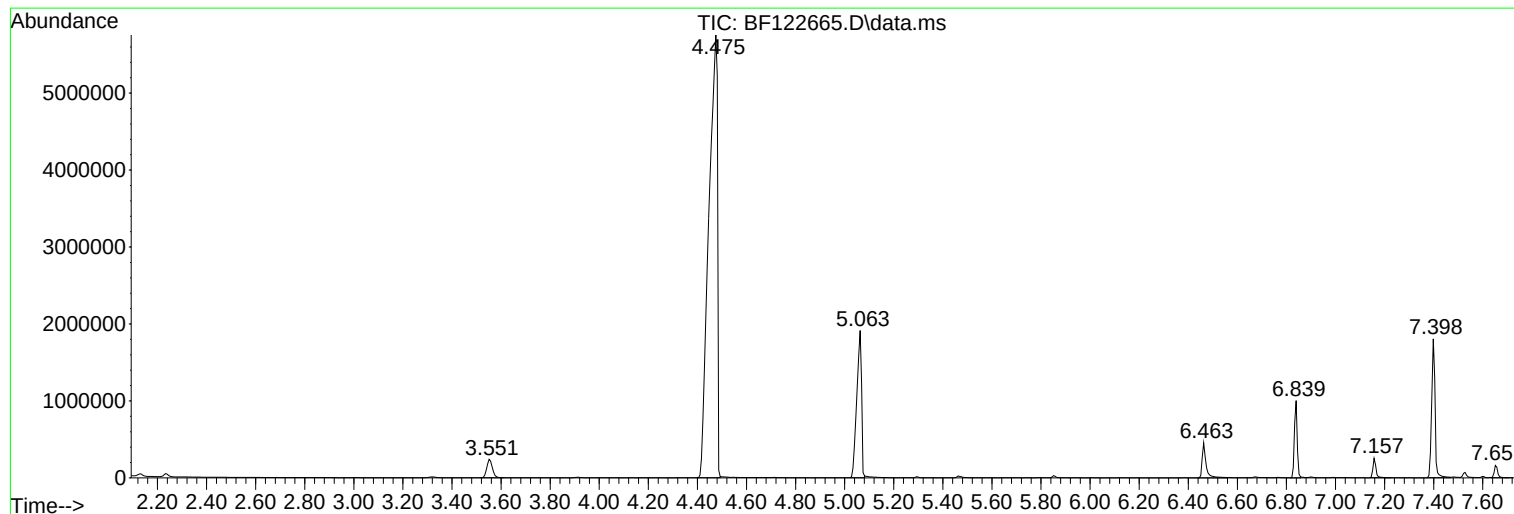
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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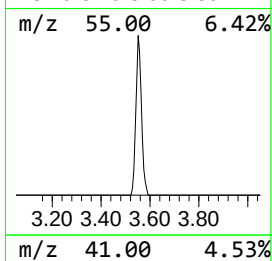
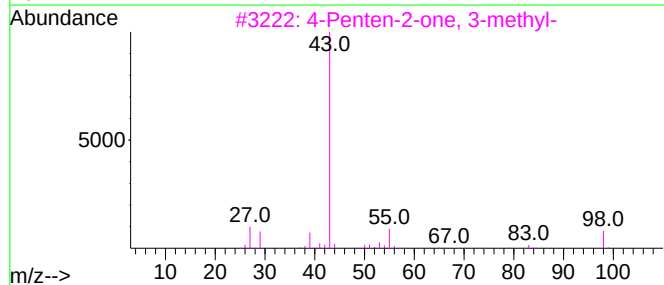
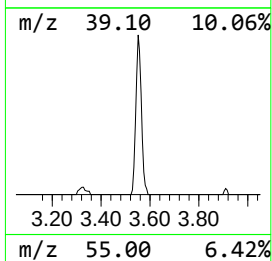
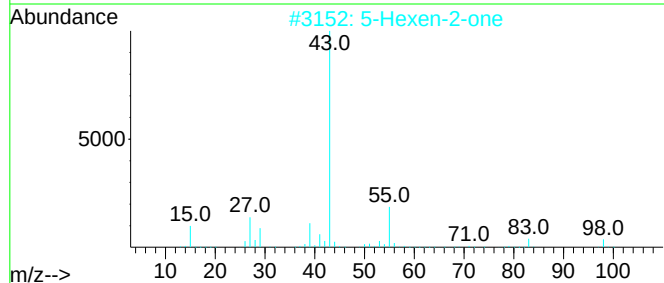
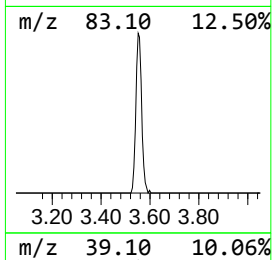
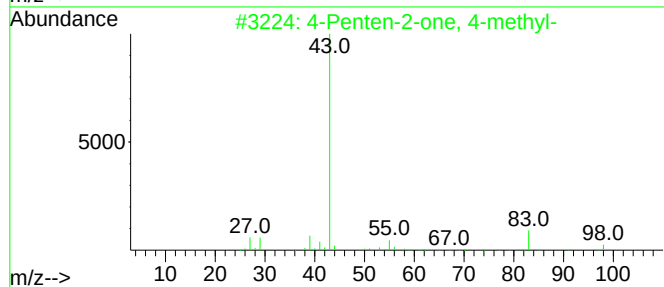
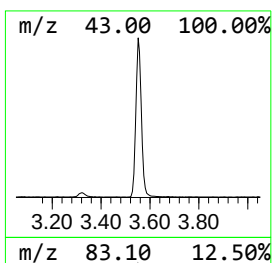
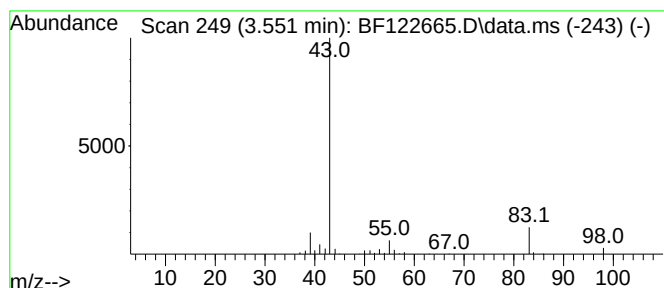
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.551	9.47 ng	376829	1,4-Dichlorobenzene-d4	6.839

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	50
4		Isoxazole, 5-methyl-	83	C4H5NO	005765-44-6	9
5		4-Hexen-2-one	98	C6H10O	025659-22-7	9



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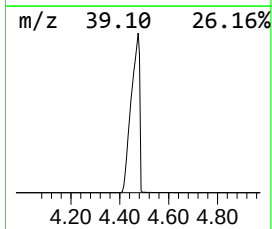
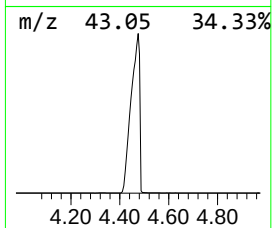
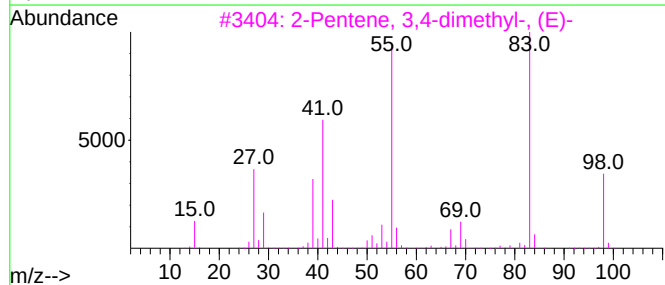
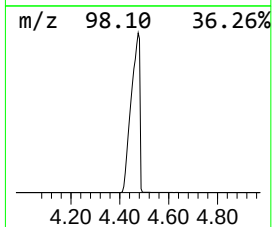
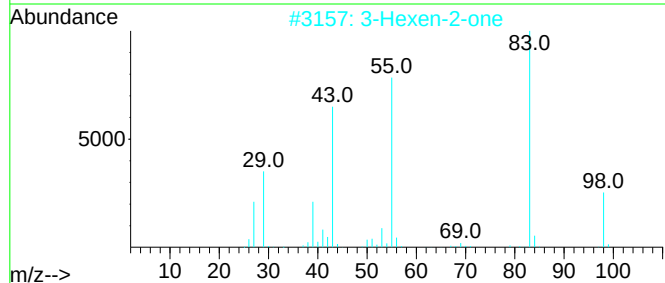
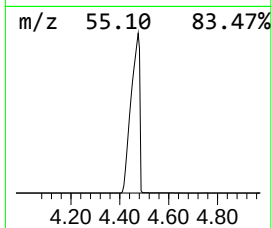
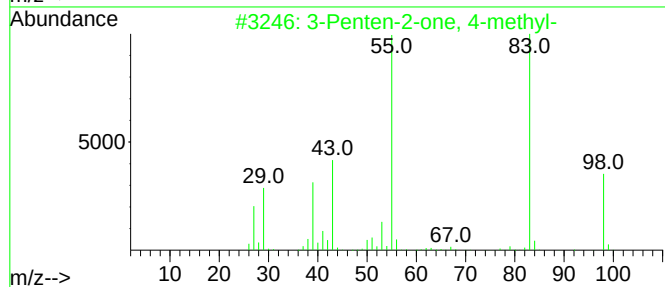
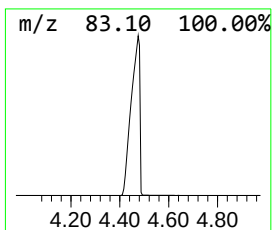
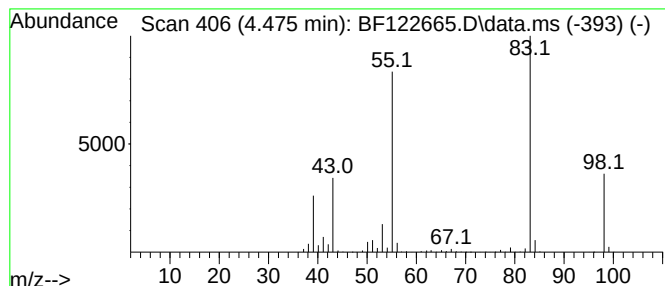
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.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.
4.475	356.25 ng	14176900	1,4-Dichlorobenzene-d4	6.839

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		2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	78



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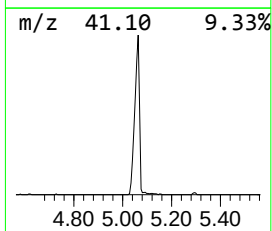
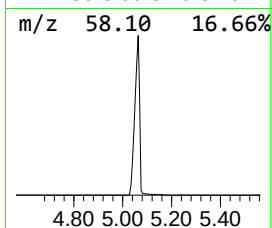
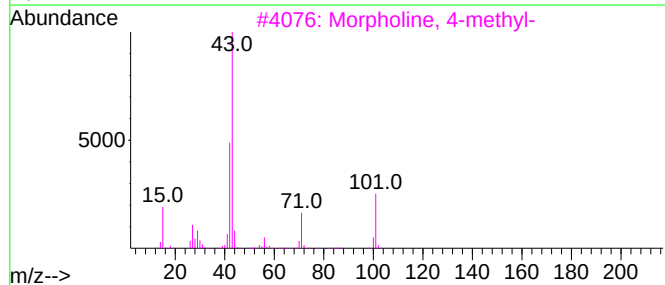
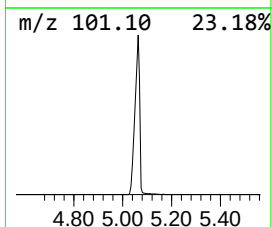
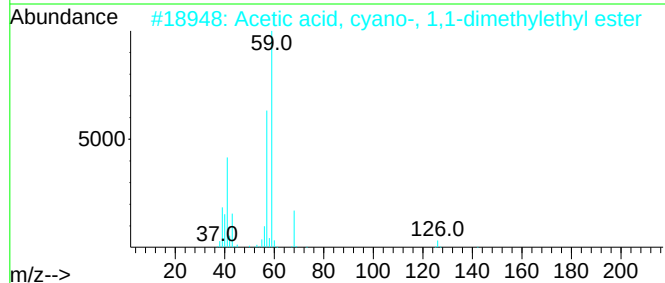
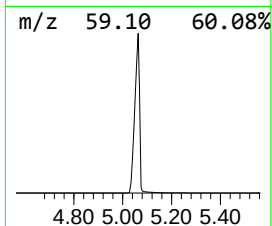
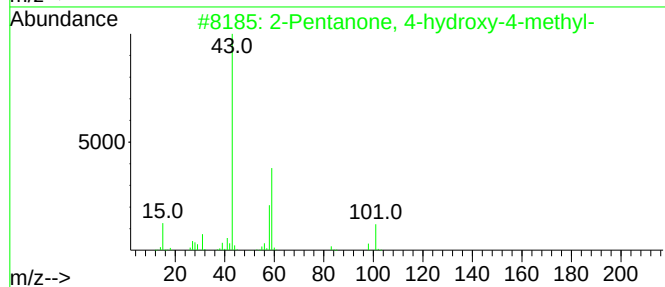
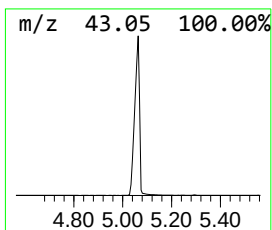
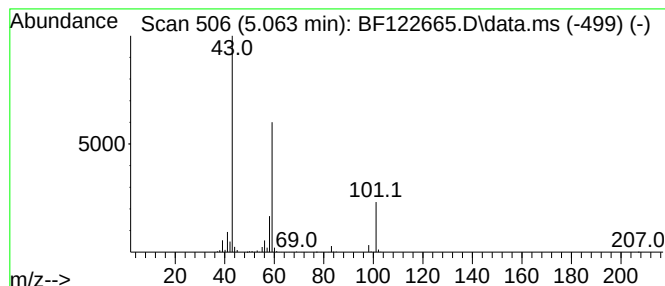
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.063	65.12 ng	2591600	1,4-Dichlorobenzene-d4	6.839

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5			5-Hexen-2-one	98	C6H10O	000109-49-9	9



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Instrument :
BNA_F
ClientSampled :
351

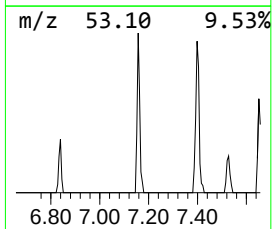
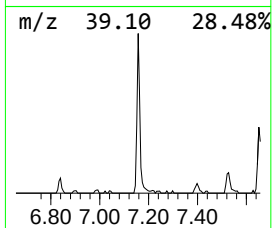
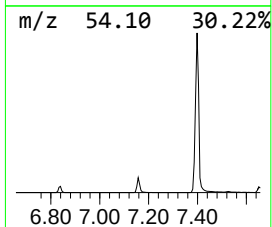
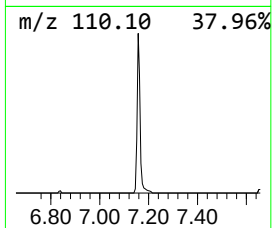
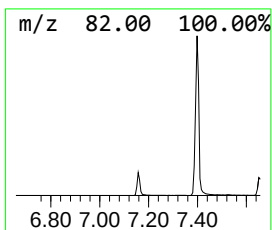
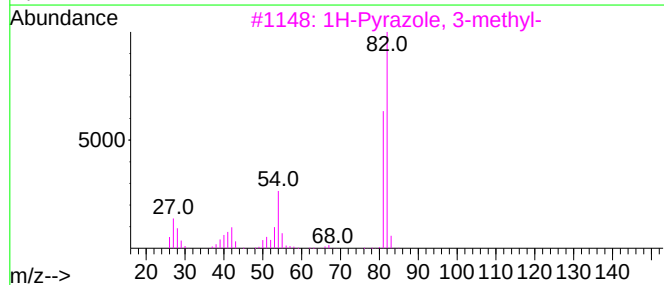
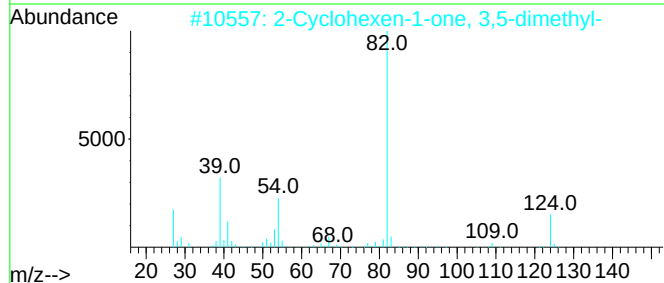
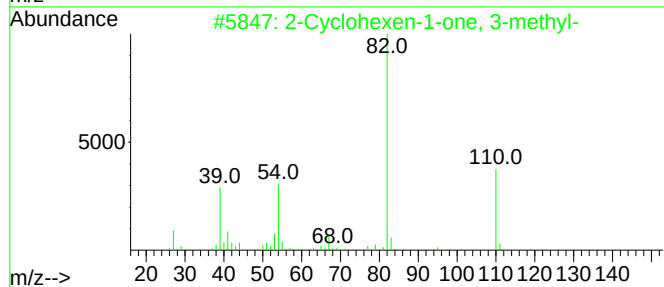
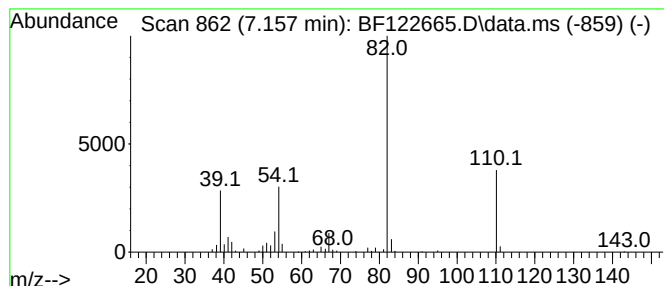
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 2-Cyclohexen-1-one, 3-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.157	5.42 ng	215498	1,4-Dichlorobenzene-d4	6.839

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Cyclohexen-1-one, 3-methyl-	110	C7H10O	001193-18-6	91
2			2-Cyclohexen-1-one, 3,5-dimethyl-	124	C8H12O	001123-09-7	64
3			1H-Pyrazole, 3-methyl-	82	C4H6N2	001453-58-3	64
4			1H-Pyrazole, 1-methyl-	82	C4H6N2	000930-36-9	53
5			2-Cyclopenten-1-one	82	C5H6O	000930-30-3	53



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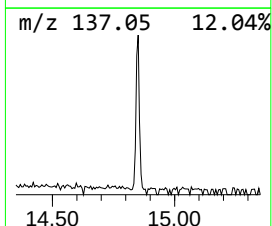
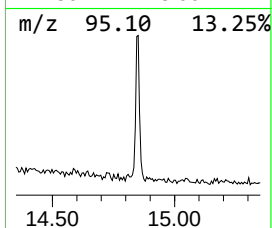
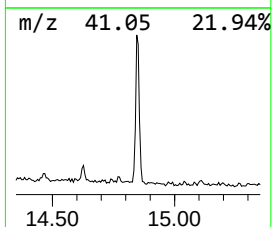
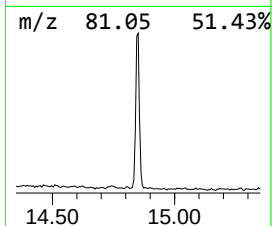
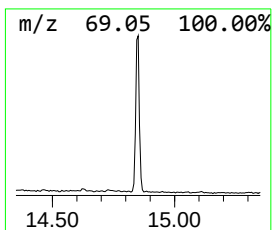
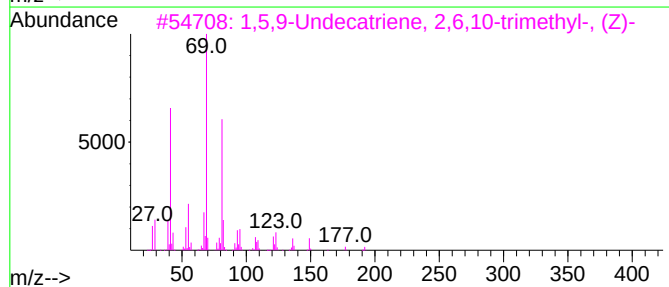
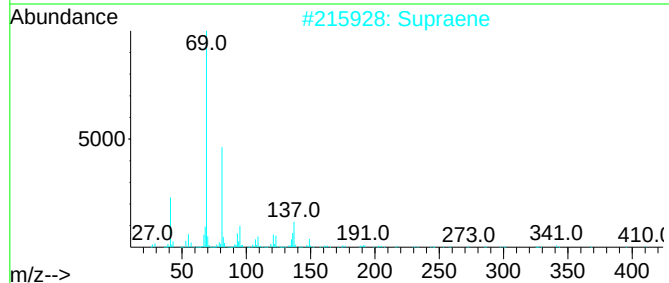
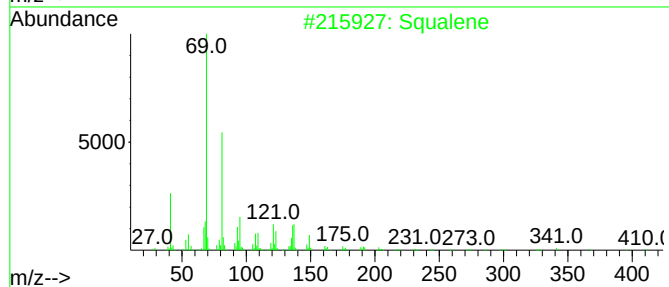
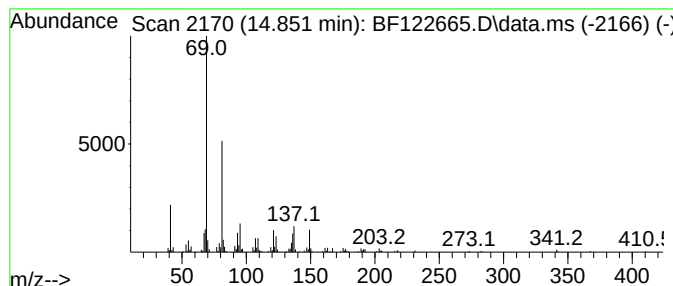
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Squalene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.851	6.24 ng	329137	Perylene-d12	15.462

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Squalene	410	C30H50	000111-02-4	99
2			Supraene	410	C30H50	007683-64-9	99
3			1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	81
4			4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	64
5			1,5,9-Decatriene, 2,3,5,8-tetram...	192	C14H24	230646-72-7	64



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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
4-Penten-2-one,...	3.551	9.5	ng	376829	1	6.839	795895	20.0
3-Penten-2-one,...	4.475	356.3	ng	14176900	1	6.839	795895	20.0
2-Pentanone, 4-...	5.063	65.1	ng	2591600	1	6.839	795895	20.0
2-Cyclohexen-1-...	7.157	5.4	ng	215498	1	6.839	795895	20.0
Squalene	14.851	6.2	ng	329137	6	15.462	1055310	20.0