

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052316\
 Data File : BF087336.D
 Acq On : 24 May 2016 11:47
 Operator : UM/SJ
 Sample : H3168-16
 Misc :
 ALS Vial : 34 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-13-COMP

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.690	6	9	54	rVB	2947538	8075157	100.00%	18.776%
2	4.890	287	289	305	rBV	166926	508600	6.30%	1.183%
3	5.530	342	345	368	rBV	2033020	3509416	43.46%	8.160%
4	7.153	484	487	494	rBV	2525269	3646200	45.15%	8.478%
5	7.267	494	497	505	rVB	2777817	3740245	46.32%	8.696%
6	7.610	524	527	538	rVB	688085	932472	11.55%	2.168%
7	7.850	545	548	558	rBV	1907607	2791920	34.57%	6.491%
8	8.525	604	607	634	rBV	1805479	2547489	31.55%	5.923%
9	9.645	702	705	718	rBV	805698	1237760	15.33%	2.878%
10	11.416	857	860	863	rBV	2727617	4089477	50.64%	9.508%
11	12.113	919	921	925	rBV	238200	309871	3.84%	0.720%
12	12.468	949	952	957	rBV	1029117	1454822	18.02%	3.383%
13	13.302	1022	1025	1028	rBV	123314	151769	1.88%	0.353%
14	13.759	1062	1065	1068	rBV	1444999	2298651	28.47%	5.345%
15	14.079	1090	1093	1098	rBV	117150	197523	2.45%	0.459%
16	14.879	1160	1163	1172	rVB	800814	1366730	16.93%	3.178%
17	16.674	1317	1320	1326	rBV	120547	161599	2.00%	0.376%
18	16.971	1344	1346	1352	rBV	110127	157767	1.95%	0.367%
19	17.211	1364	1367	1370	rBV	3025532	3531499	43.73%	8.211%
20	18.548	1482	1484	1487	rBV	650942	1030334	12.76%	2.396%
21	18.606	1487	1489	1495	rVB2	114405	207147	2.57%	0.482%
22	19.577	1571	1574	1580	rBV	132400	172180	2.13%	0.400%
23	19.680	1580	1583	1586	rVV	82444	89073	1.10%	0.207%
24	19.840	1595	1597	1603	rBV	38367	86741	1.07%	0.202%
25	20.217	1629	1630	1636	rVB	459819	714464	8.85%	1.661%

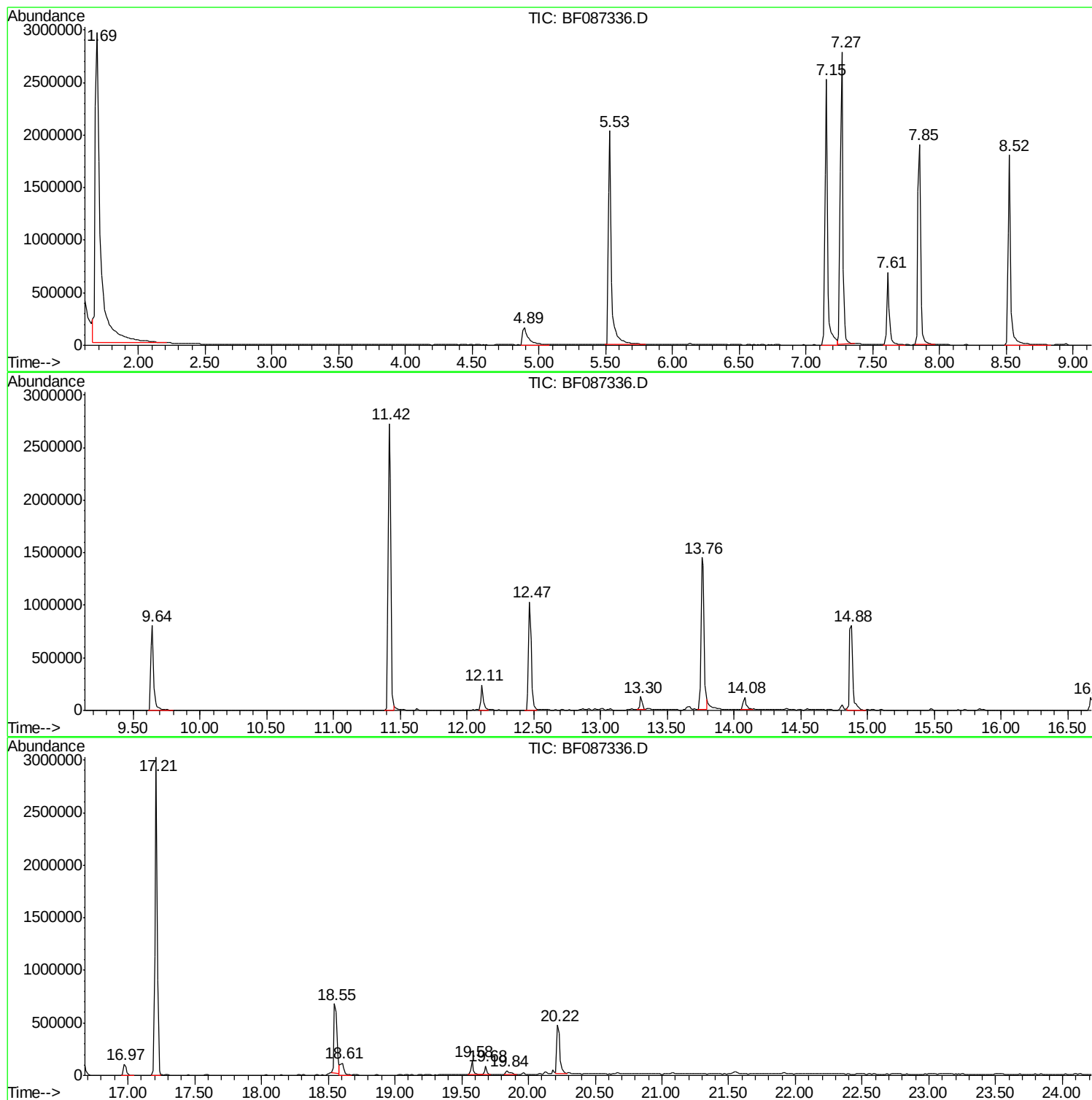
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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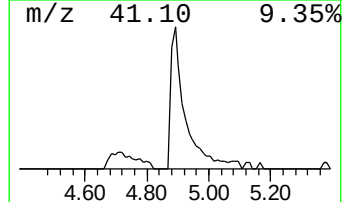
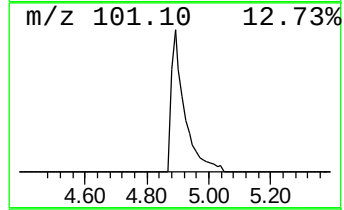
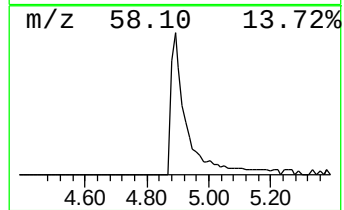
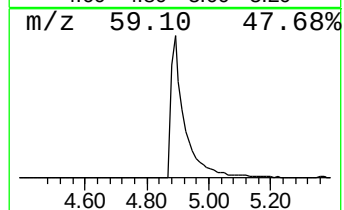
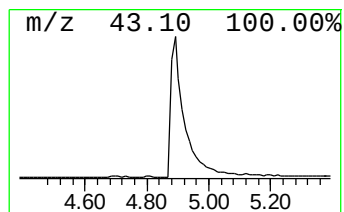
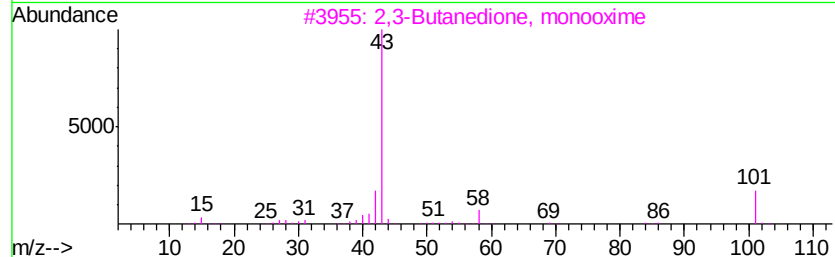
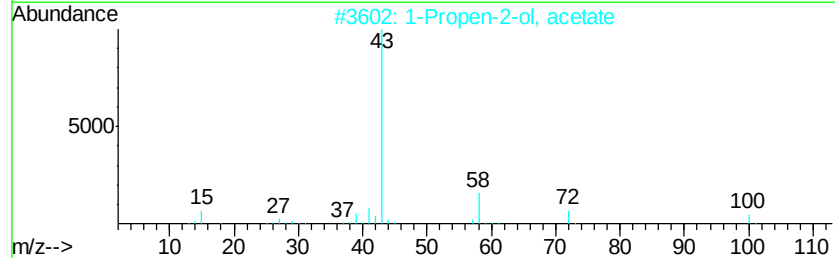
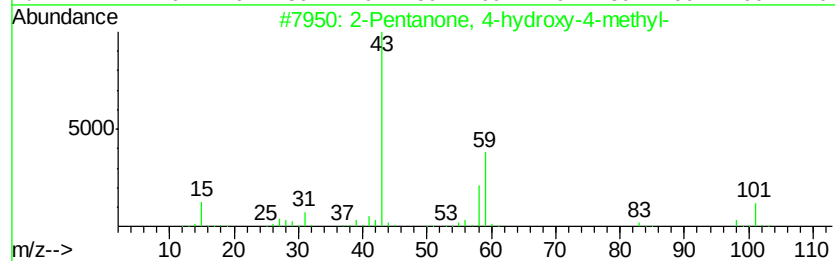
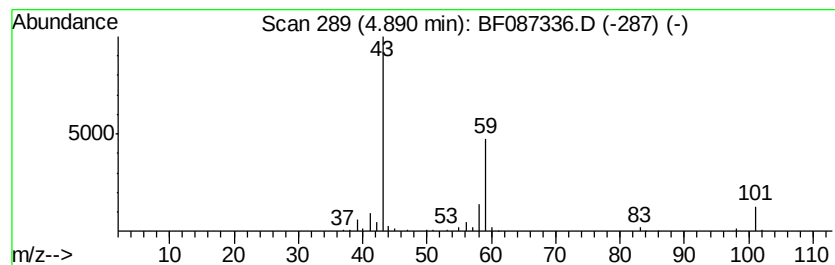
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.89	10.91 ng	508600	1,4-Dichlorobenzene-d4	7.61

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	38
2			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4			dl-4-Amino-3-hydroxybutyric acid	119	C4H9NO3	000352-21-6	9
5			Acetic acid, 2-propenyl ester	100	C5H8O2	000591-87-7	9



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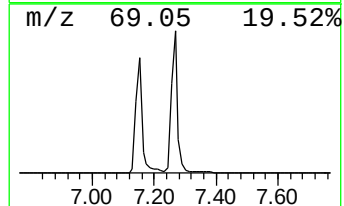
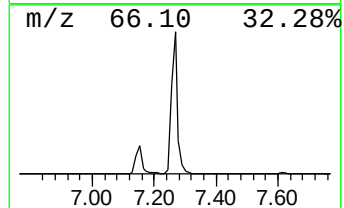
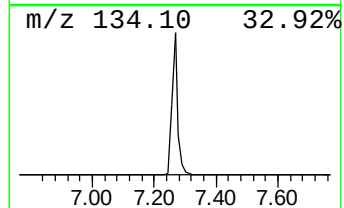
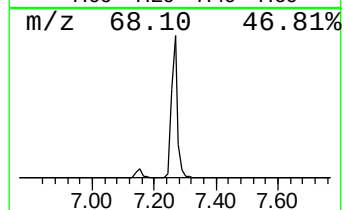
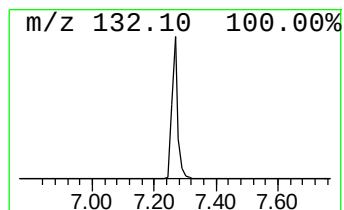
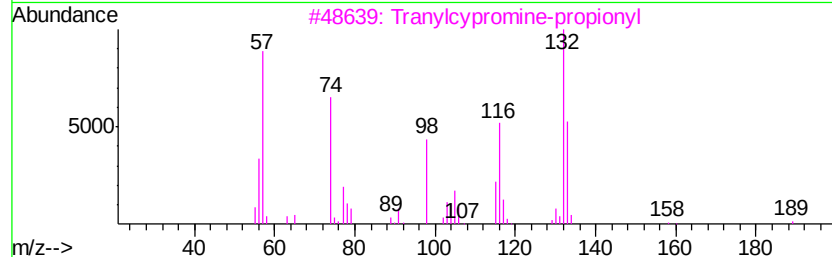
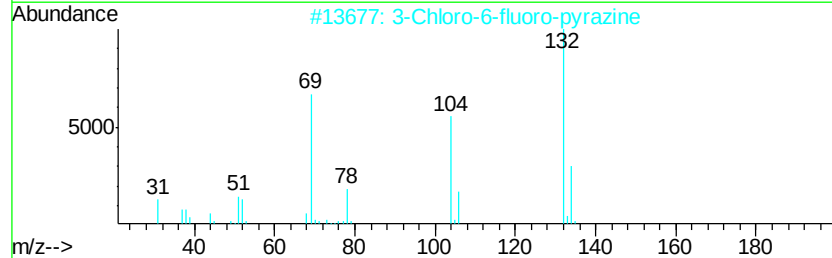
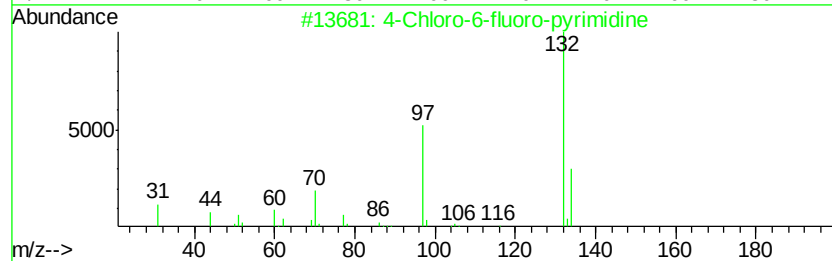
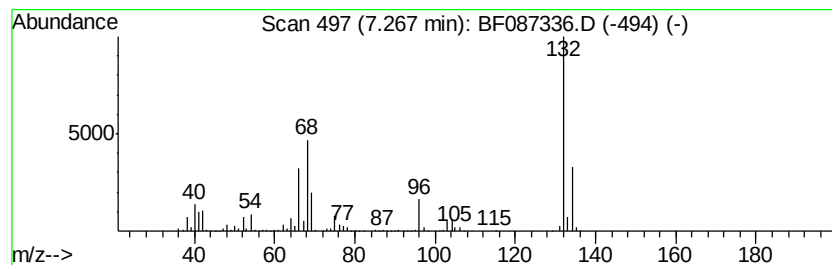
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Peak Number 3 unknown7.27 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.27	80.22 ng	3740250	1,4-Dichlorobenzene-d4	7.61

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	22
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12



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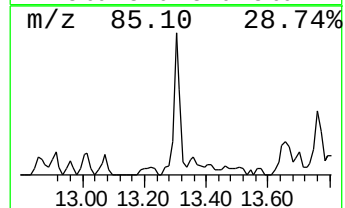
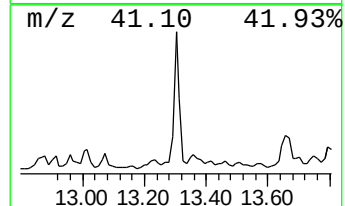
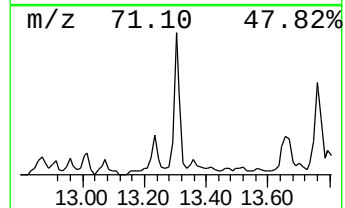
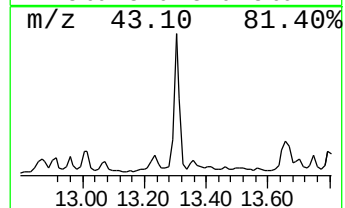
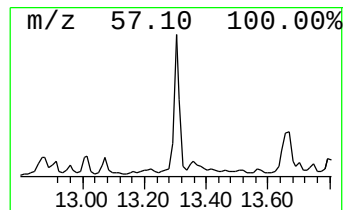
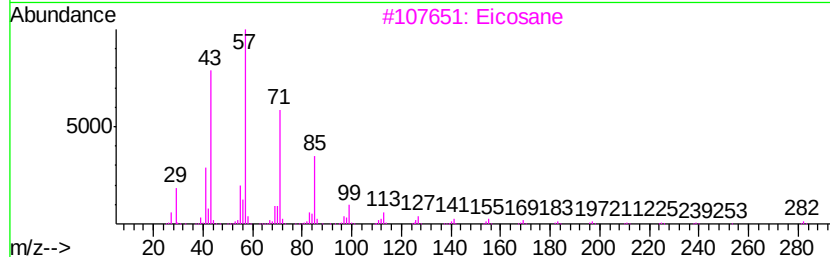
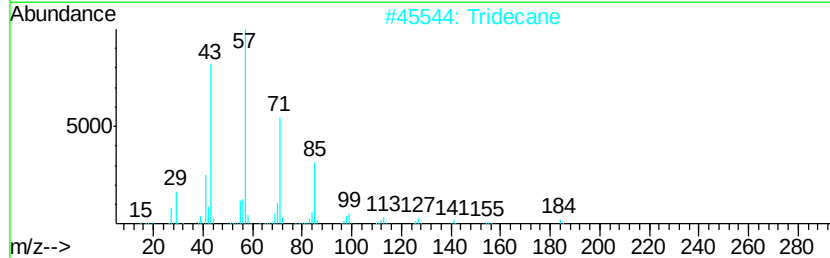
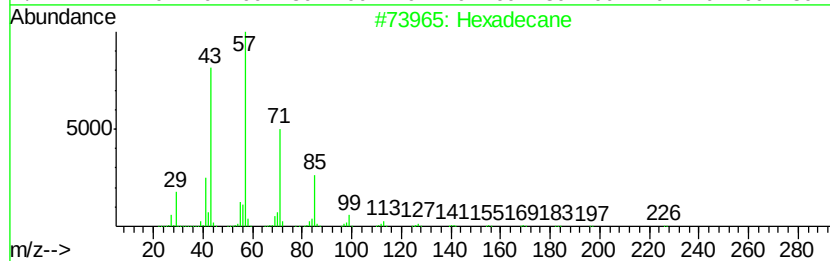
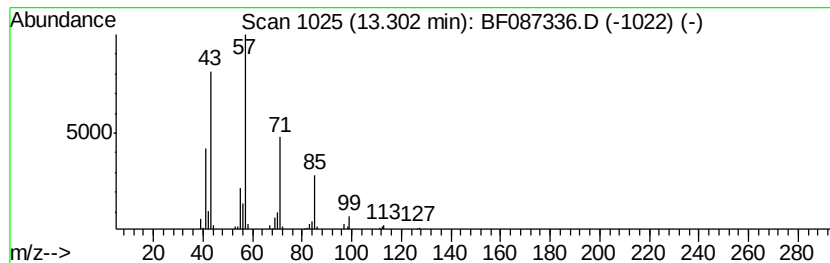
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Peak Number 5 Hexadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.30	2.09 ng	151769	Acenaphthene-d10	12.47	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	91
2	Tridecane	184	C13H28	000629-50-5	90
3	Eicosane	282	C20H42	000112-95-8	78
4	Heptadecane	240	C17H36	000629-78-7	72
5	Tetradecane	198	C14H30	000629-59-4	72



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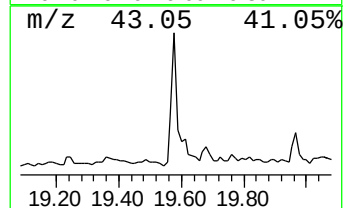
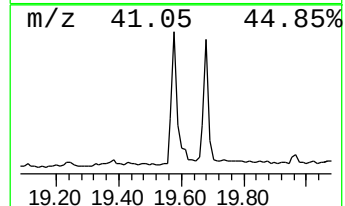
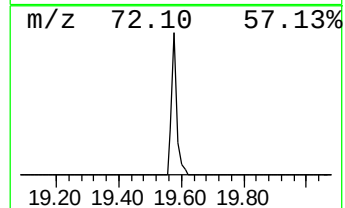
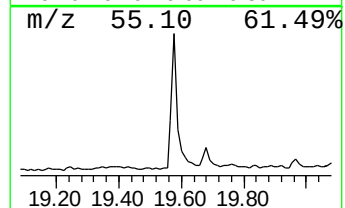
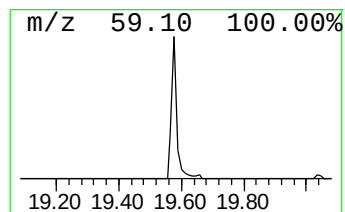
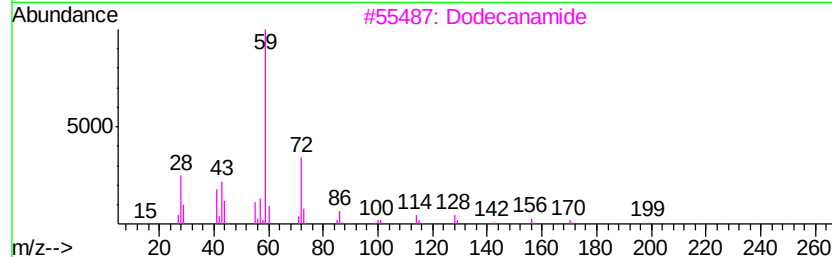
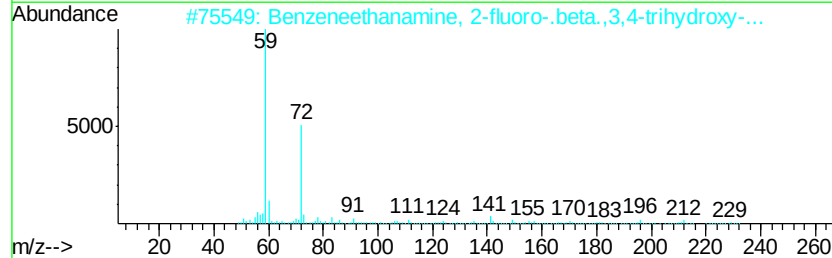
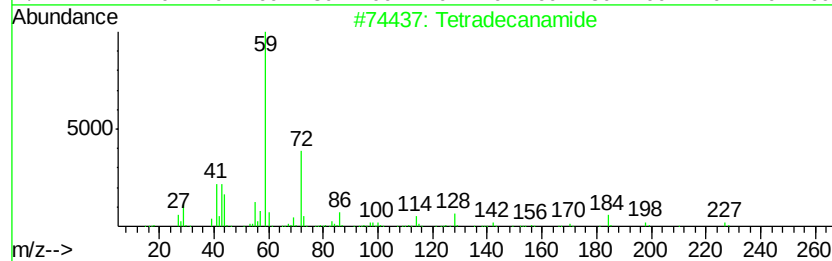
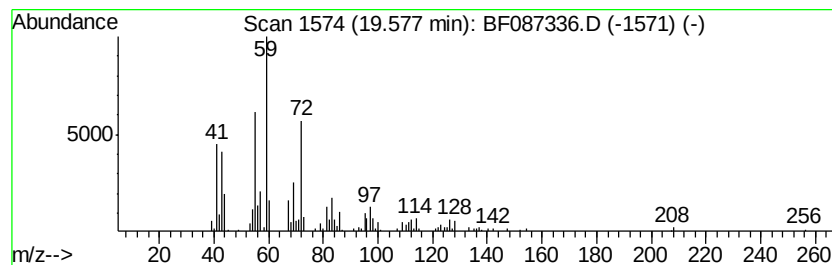
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 7 Tetradecanamide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.58	4.82 ng	172180	Perylene-d12	20.22	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanamide	227	C14H29NO	000638-58-4	59
2	Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	59
3	Dodecanamide	199	C12H25NO	001120-16-7	53
4	Pentadecanamide, 15-bromo-	319	C15H30BrNO	1000163-86-1	50
5	Hexadecanamide	255	C16H33NO	000629-54-9	50



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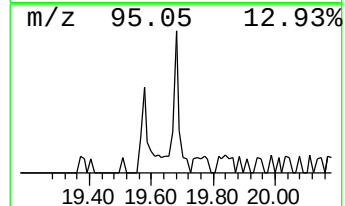
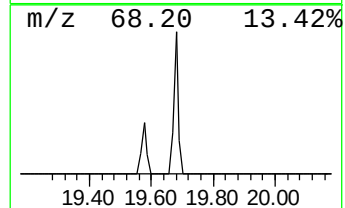
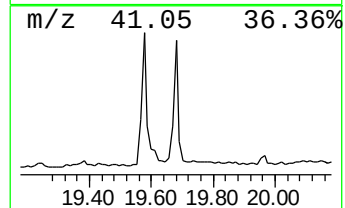
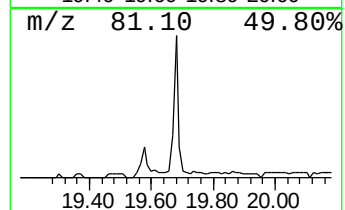
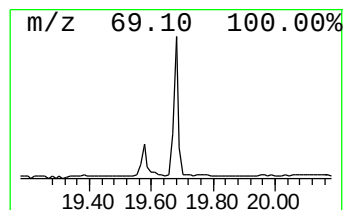
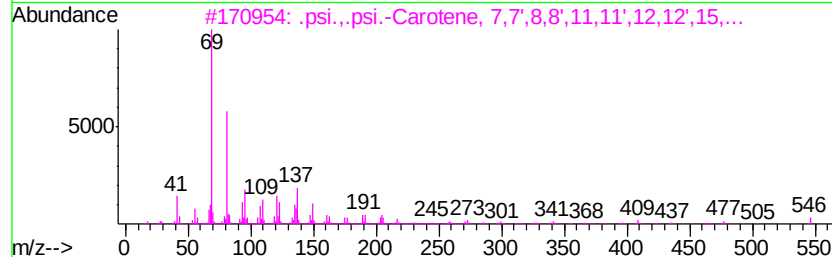
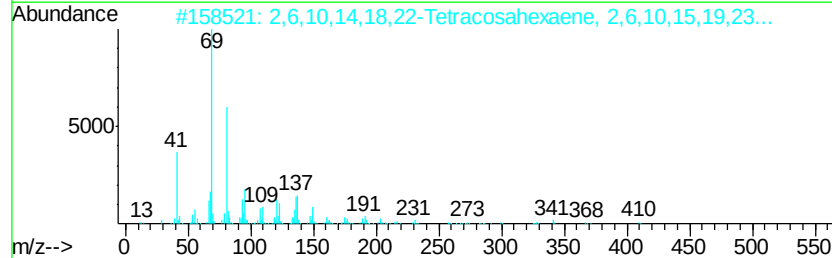
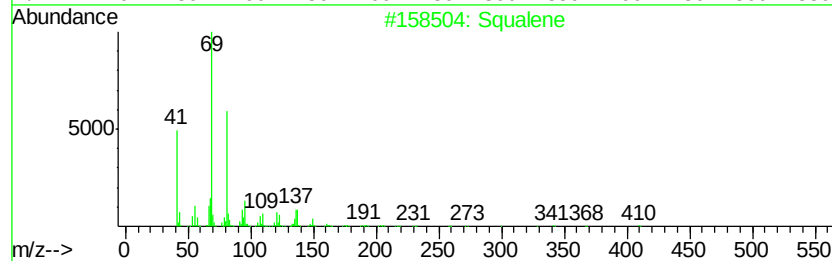
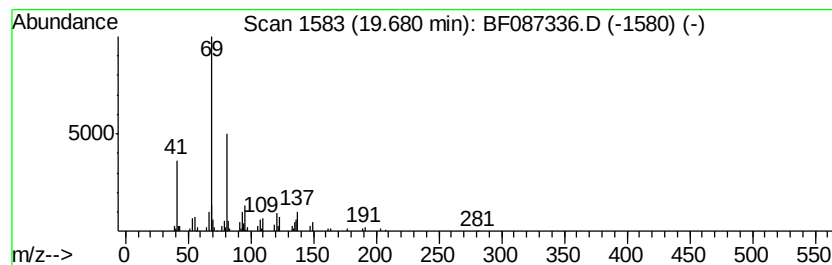
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 8 Squalene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.68	2.49 ng	89073	Perylene-d12	20.22

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	007683-64-9	91
2		2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	90
3		.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	83
4		2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	000106-28-5	78
5		Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	78



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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.89	10.9	ng	508600	1	7.61	932472	20.0
unknown7.27	7.27	80.2	ng	3740250	1	7.61	932472	20.0
Hexadecane	13.30	2.1	ng	151769	3	12.47	1454820	20.0
Tetradecanamide	19.58	4.8	ng	172180	6	20.22	714464	20.0
Squalene	19.68	2.5	ng	89073	6	20.22	714464	20.0