

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052016\
 Data File : BF087269.D
 Acq On : 21 May 2016 13:29
 Operator : UM/SJ
 Sample : H3169-14
 Misc :
 ALS Vial : 40 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-03-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-BF051716.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	1.701	8	10	43	rVB	2137106	4044796	100.00%	11.657%
2	4.673	268	270	284	rBV	253445	507977	12.56%	1.464%
3	5.142	308	311	331	rBV	2357937	2904168	71.80%	8.369%
4	6.227	403	406	408	rBV	2822359	3132644	77.45%	9.028%
5	6.330	413	415	418	rBV	2562412	2991558	73.96%	8.621%
6	6.559	432	435	441	rVB	614683	871384	21.54%	2.511%
7	6.707	446	448	455	rVV	2504622	2271971	56.17%	6.548%
8	7.130	483	485	498	rBV	2058391	2017048	49.87%	5.813%
9	7.839	545	547	550	rBV	1132723	1187485	29.36%	3.422%
10	8.925	639	642	644	rBV	3180112	3508002	86.73%	10.110%
11	9.325	675	677	681	rBV	535758	461890	11.42%	1.331%
12	9.531	693	695	697	rBV	77901	74767	1.85%	0.215%
13	9.588	697	700	702	rBV	1578356	1372384	33.93%	3.955%
14	10.033	737	739	740	rVB	132230	114999	2.84%	0.331%
15	10.251	754	758	761	rBV	42773	71371	1.76%	0.206%
16	10.376	766	769	778	rVV	2005704	2032252	50.24%	5.857%
17	10.502	778	780	787	rVB	148693	197810	4.89%	0.570%
18	10.696	795	797	801	rBV	21047	40614	1.00%	0.117%
19	10.948	817	819	820	rBV	99254	91457	2.26%	0.264%
20	11.062	827	829	834	rBV	1339303	1354593	33.49%	3.904%
21	11.371	854	856	858	rVB	48908	40803	1.01%	0.118%
22	12.274	933	935	942	rBV	144422	147826	3.65%	0.426%
23	12.502	951	955	957	rBV	123047	151988	3.76%	0.438%
24	12.651	965	968	970	rBV	2590941	3022499	74.73%	8.710%
25	13.588	1044	1050	1056	rBV5	25224	98531	2.44%	0.284%
26	13.691	1056	1059	1065	rVB	978570	1076481	26.61%	3.102%
27	14.445	1122	1125	1129	rBV	70615	92795	2.29%	0.267%
28	14.525	1129	1132	1135	rVB	68793	70371	1.74%	0.203%
29	14.697	1145	1147	1150	rBV	29430	49880	1.23%	0.144%
30	15.040	1175	1177	1187	rVB	555073	699350	17.29%	2.015%

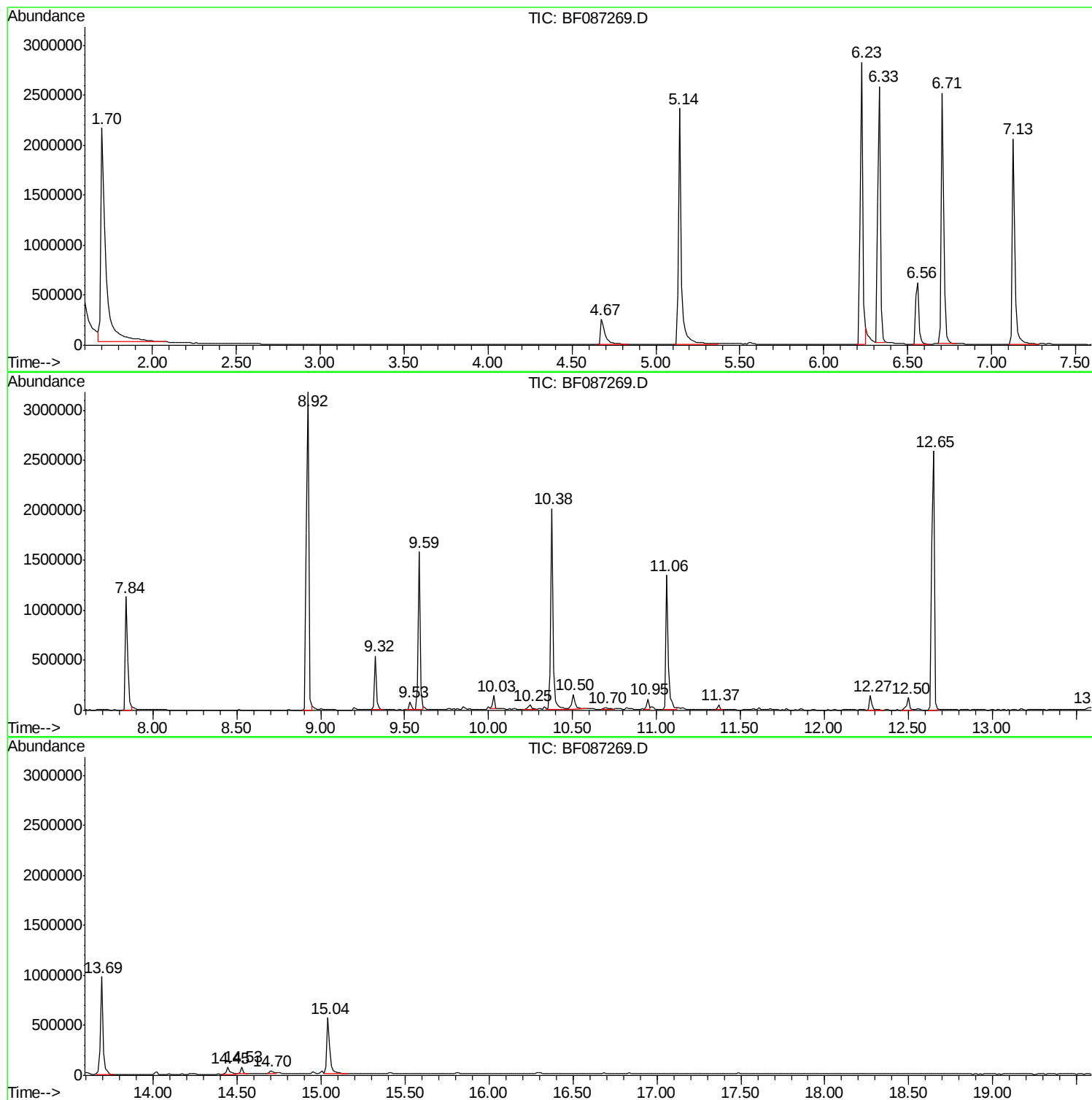
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF051716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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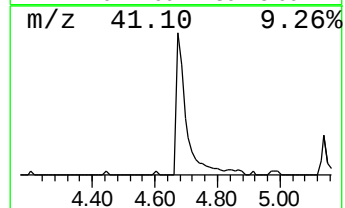
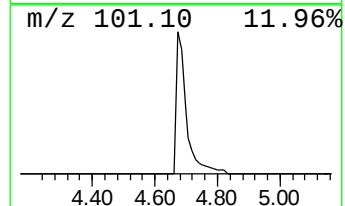
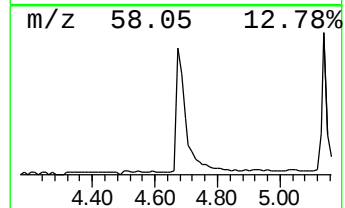
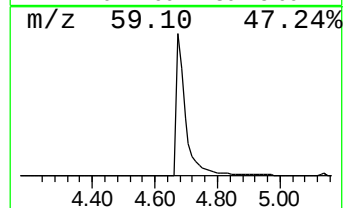
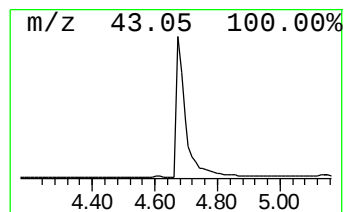
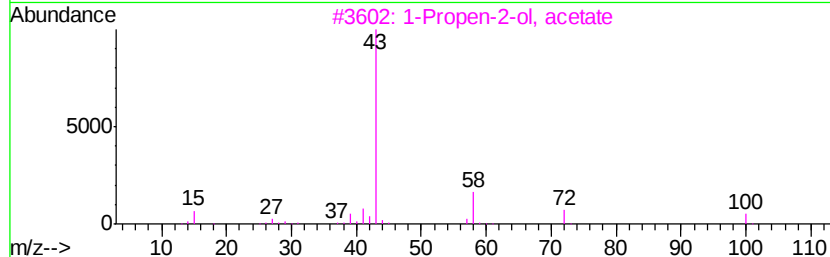
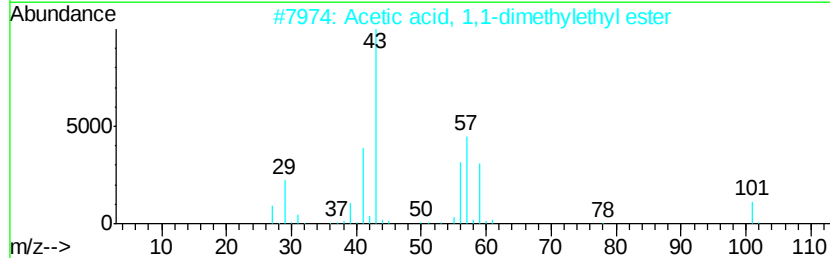
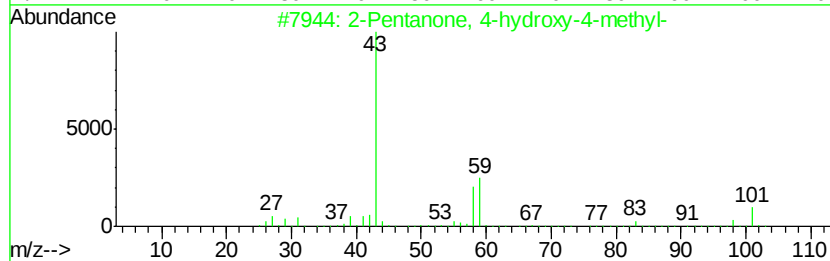
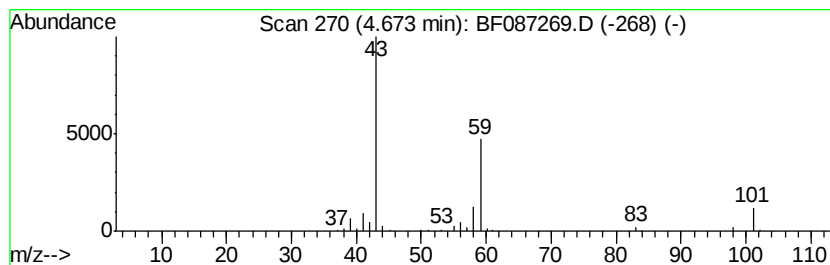
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.67	11.66 ng	507977	1,4-Dichlorobenzene-d4	6.56

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, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	23		
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		
4	Diacetamide	101	C4H7NO2	000625-77-4	9		
5	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9		



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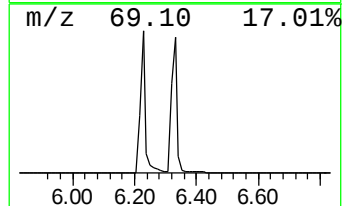
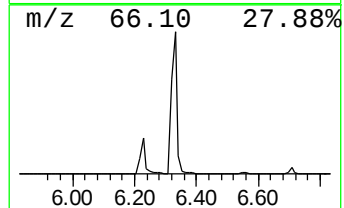
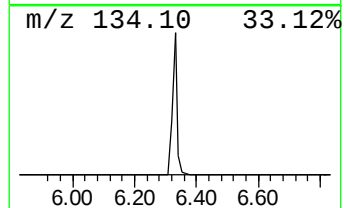
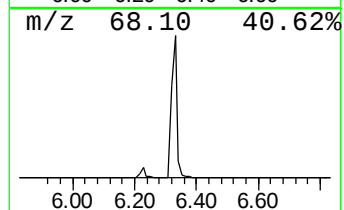
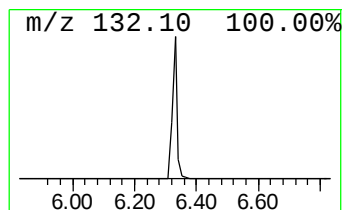
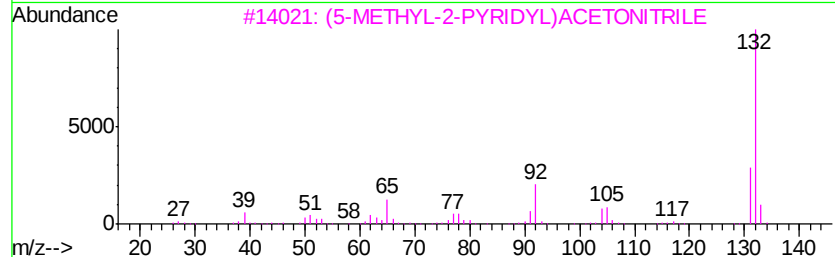
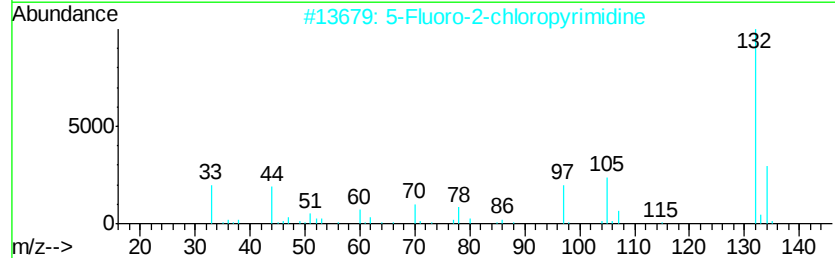
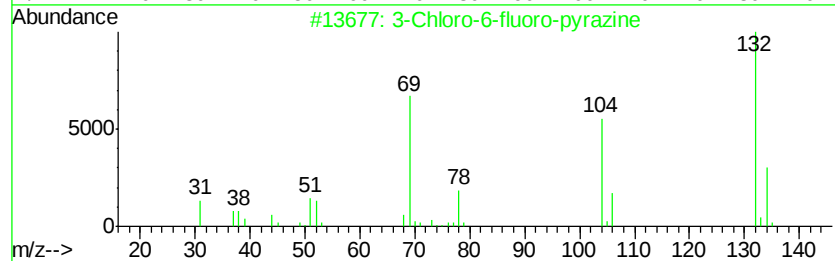
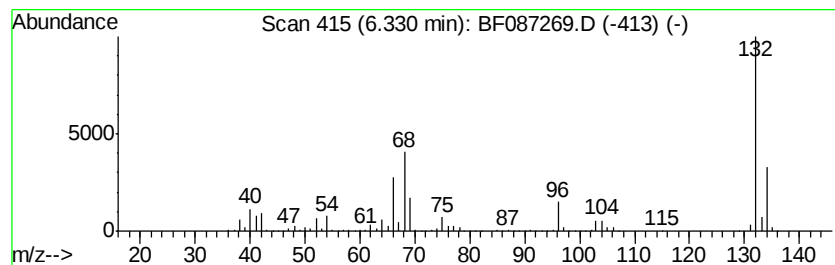
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Peak Number 3 unknown6.33 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.33	68.66 ng	2991560	1,4-Dichlorobenzene-d4	6.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3		(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
4		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5		Benzene, 1,2,4-trifluoro-	132	C6H3F3	000367-23-7	9



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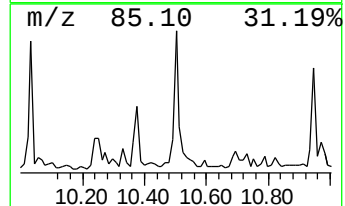
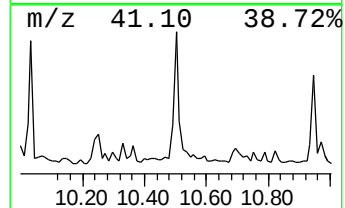
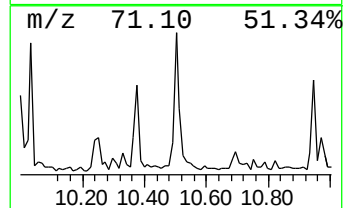
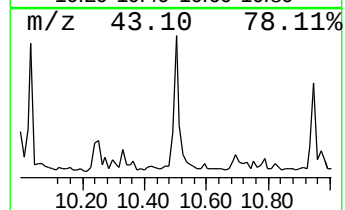
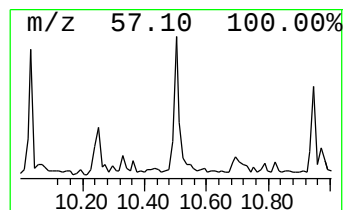
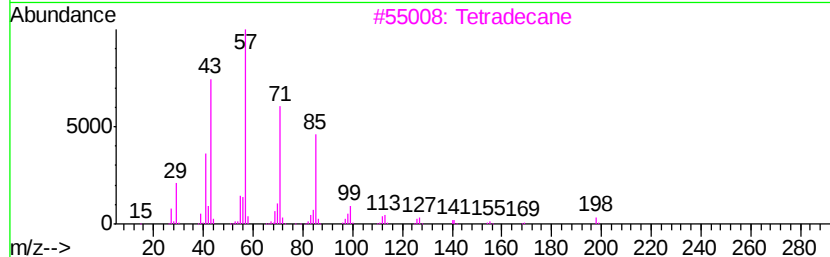
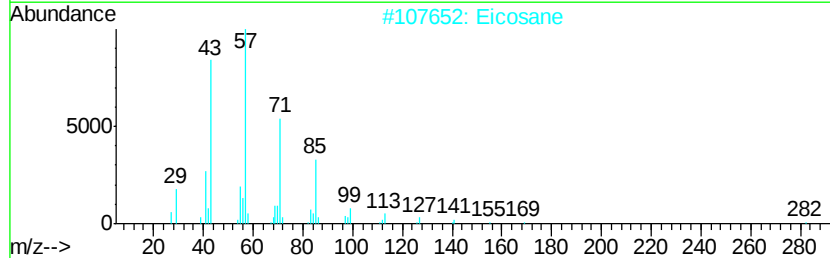
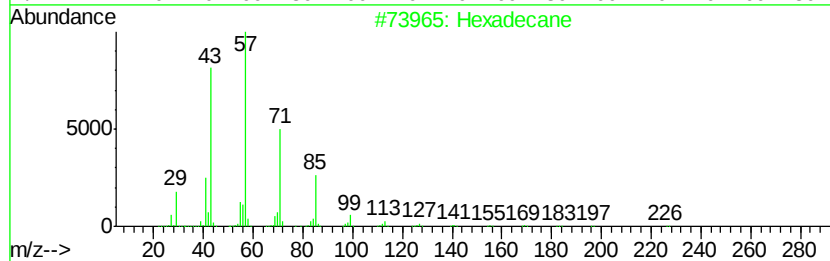
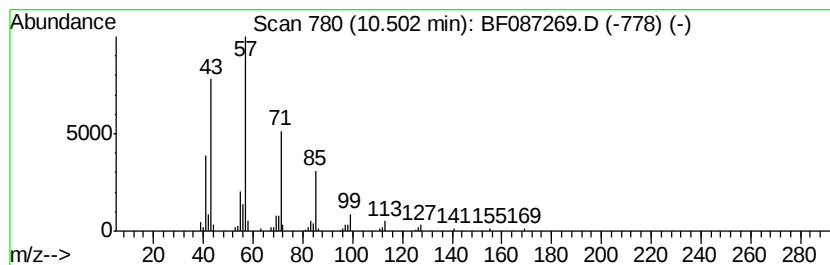
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Peak Number 5 Hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.50	2.92 ng	197810	Phenanthrene-d10	11.06	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	91
2	Eicosane	282	C20H42	000112-95-8	91
3	Tetradecane	198	C14H30	000629-59-4	83
4	Pentadecane	212	C15H32	000629-62-9	78
5	Dodecane, 3-methyl-	184	C13H28	017312-57-1	72



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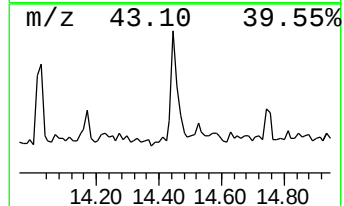
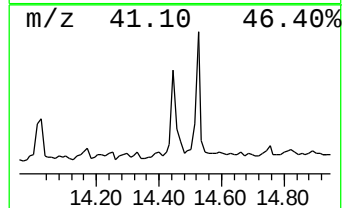
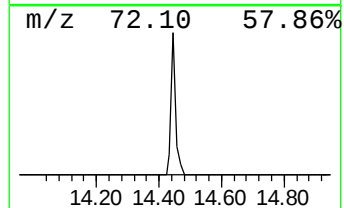
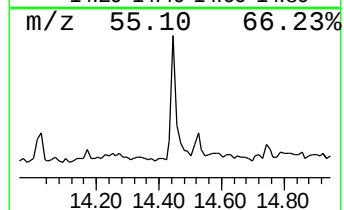
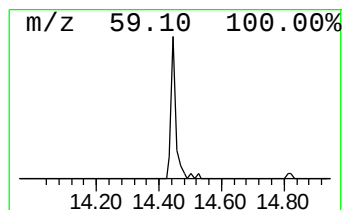
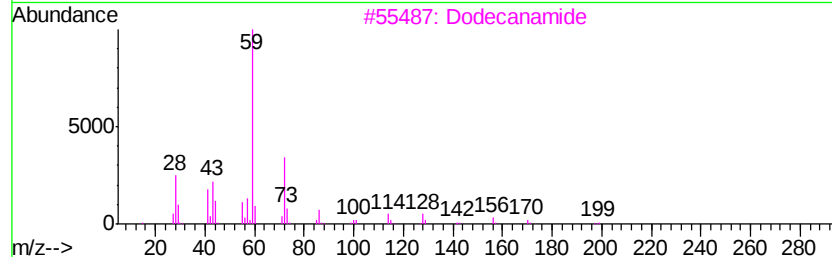
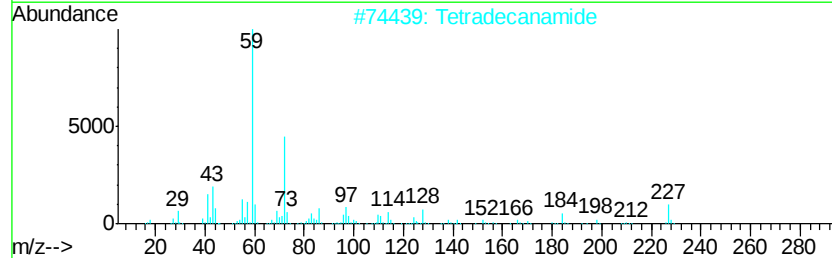
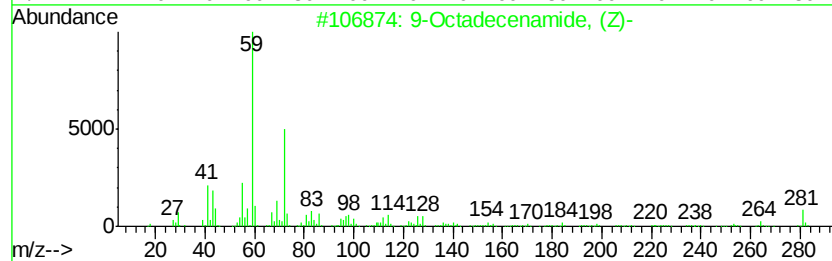
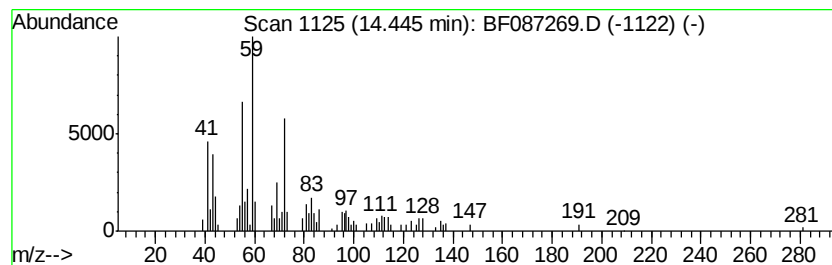
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Peak Number 6 9-Octadecenamide, (Z)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.45	2.65 ng	92795	Perylene-d12	15.04

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	83
2		Tetradecanamide	227	C14H29NO	000638-58-4	80
3		Dodecanamide	199	C12H25NO	001120-16-7	64
4		Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	53
5		7-Nonenamide	155	C9H17NO	090949-53-4	53



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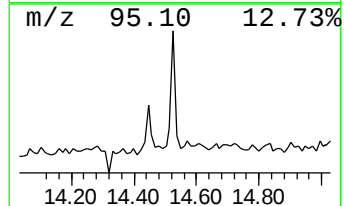
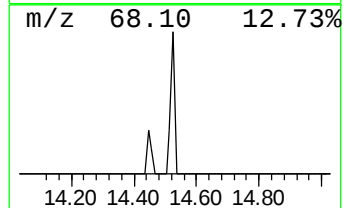
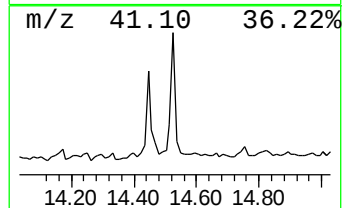
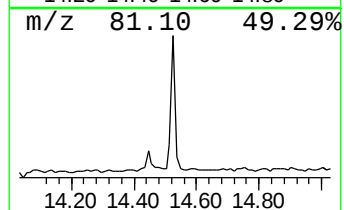
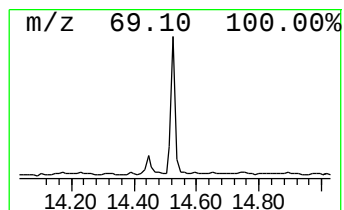
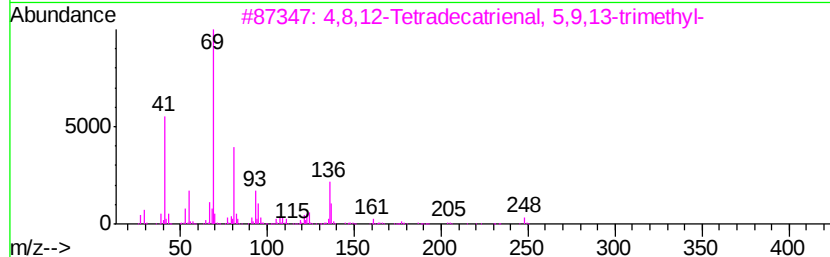
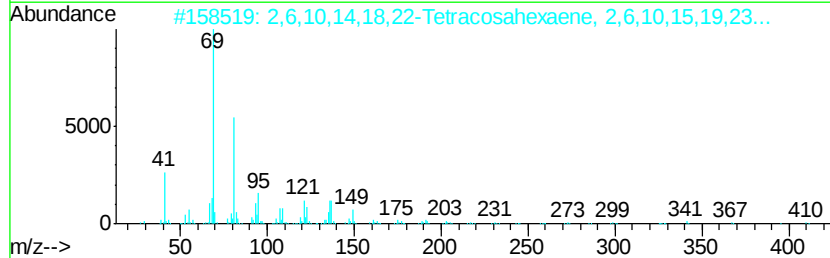
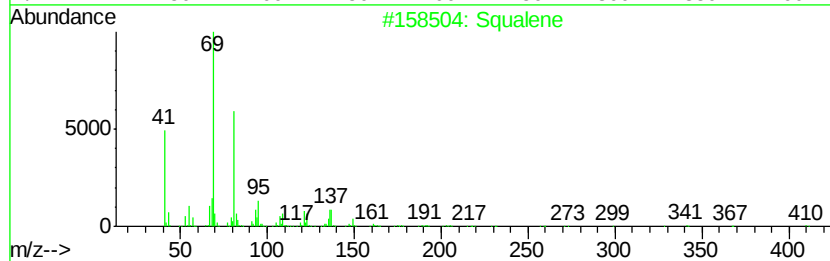
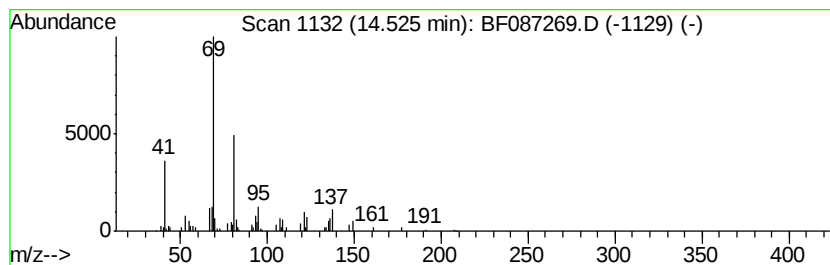
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 7 Squalene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.53	2.01 ng	70371	Perylene-d12	15.04

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	86
3		4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	78
4		2,6,10-Dodecatrien-1-ol, 3,7,11-...	264	C17H28O2	004128-17-0	64
5		1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	64



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.67	11.7	ng	507977	1	6.56	871384	20.0
unknown6.33	6.33	68.7	ng	2991560	1	6.56	871384	20.0
Hexadecane	10.50	2.9	ng	197810	4	11.06	1354590	20.0
9-Octadecenamide, ...	14.45	2.6	ng	92795	6	15.04	699350	20.0
Squalene	14.53	2.0	ng	70371	6	15.04	699350	20.0