

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061616\
 Data File : BF088081.D
 Acq On : 16 Jun 2016 17:52
 Operator : UM/SJ
 Sample : H3570-14
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-16-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-BF060716.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	1.644	3	5	7	rVB	60053	87162	3.14%	0.414%
2	1.690	7	9	17	rVB	148813	329475	11.87%	1.564%
3	1.804	17	19	27	rBV	1710940	2775691	100.00%	13.179%
4	4.879	286	288	297	rBV	63497	101409	3.65%	0.481%
5	5.301	323	325	328	rBV	1419562	1469628	52.95%	6.978%
6	6.364	415	418	420	rBV	1225382	1664883	59.98%	7.905%
7	6.479	426	428	431	rBV	1350451	1615230	58.19%	7.669%
8	6.719	447	449	451	rBV	738899	655582	23.62%	3.113%
9	6.867	460	462	465	rVB	1084782	1288286	46.41%	6.117%
10	7.279	496	498	501	rBV	778432	1033035	37.22%	4.905%
11	7.999	559	561	564	rBV	853090	851519	30.68%	4.043%
12	9.085	653	656	658	rBV	1701604	1931460	69.58%	9.171%
13	9.473	688	690	692	rVB	404362	422878	15.24%	2.008%
14	9.690	707	709	712	rBV	24963	28278	1.02%	0.134%
15	9.748	712	714	717	rVV	773271	934181	33.66%	4.436%
16	10.193	751	753	755	rVB	74101	55881	2.01%	0.265%
17	10.411	769	772	775	rBV	23172	36800	1.33%	0.175%
18	10.536	781	783	786	rBV	1098643	1053664	37.96%	5.003%
19	10.662	792	794	798	rBV	84373	95185	3.43%	0.452%
20	11.108	831	833	835	rBV	46124	42303	1.52%	0.201%
21	11.233	842	844	846	rBV	1056437	988773	35.62%	4.695%
22	12.285	932	936	942	rBV	27547	48949	1.76%	0.232%
23	12.434	947	949	951	rBV	33251	34346	1.24%	0.163%
24	12.662	965	969	971	rBV	41403	72886	2.63%	0.346%
25	12.811	980	982	985	rBV	1477265	1515813	54.61%	7.197%
26	13.714	1059	1061	1071	rBV	55612	122000	4.40%	0.579%
27	13.862	1071	1074	1076	rBV	766090	809313	29.16%	3.843%
28	14.342	1113	1116	1123	rBV3	15079	48999	1.77%	0.233%
29	14.617	1137	1140	1144	rBV	57346	81159	2.92%	0.385%
30	14.868	1159	1162	1166	rBV	18491	32596	1.17%	0.155%
31	15.245	1193	1195	1198	rBV	556474	667530	24.05%	3.169%
32	17.211	1363	1367	1374	rBV5	14830	60428	2.18%	0.287%
33	17.428	1383	1386	1398	rVB	32649	106010	3.82%	0.503%

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Integration Parameters: rteint.p
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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

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Peak separation: 5

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

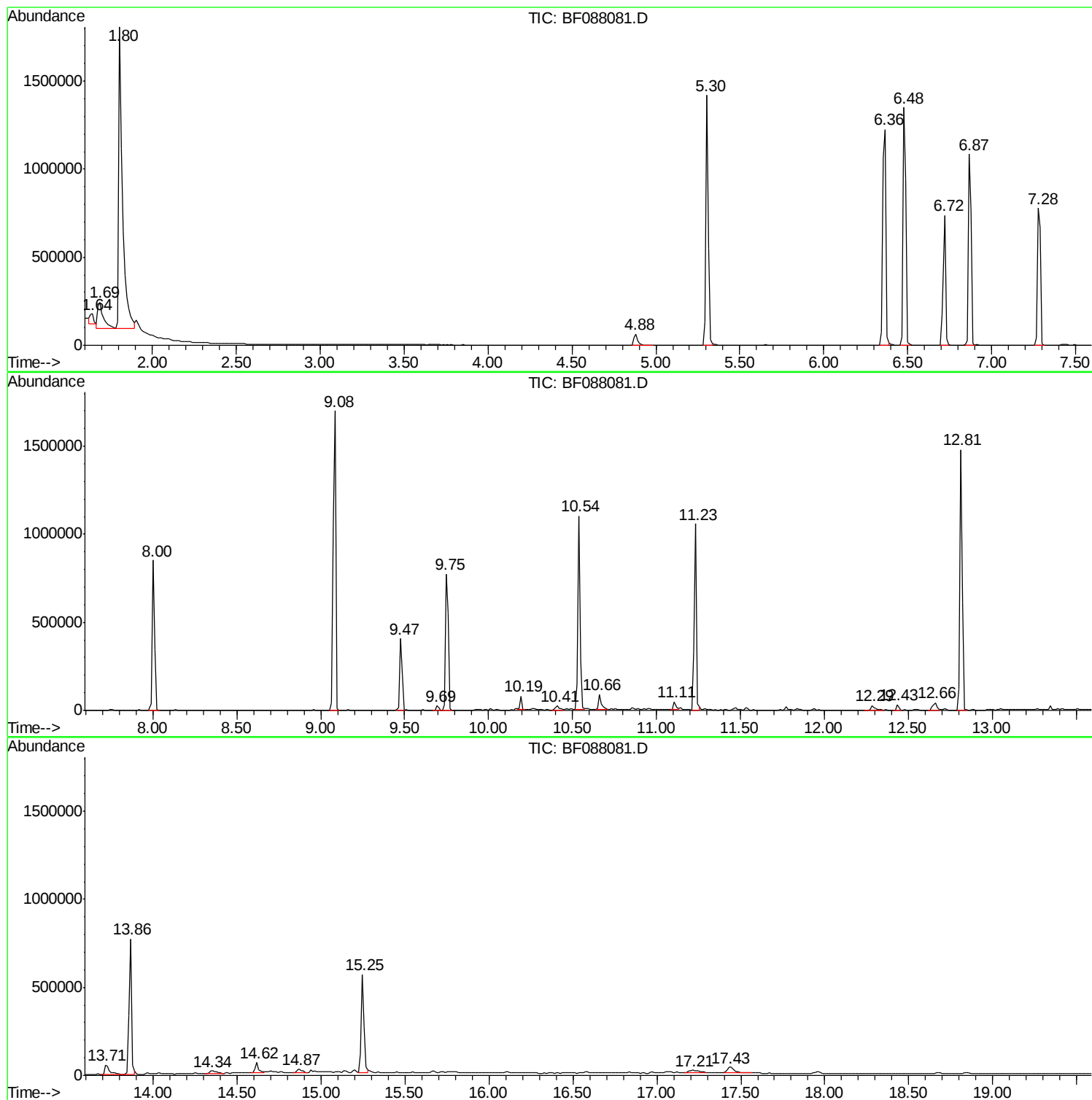
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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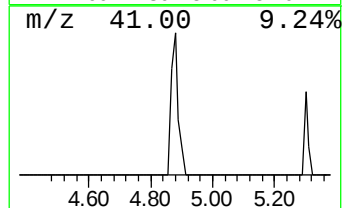
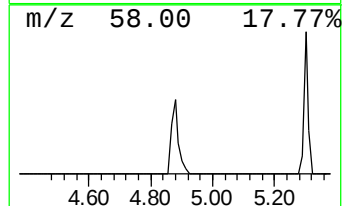
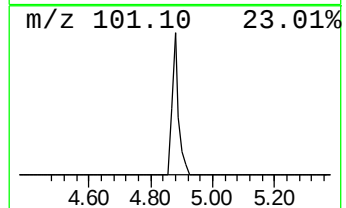
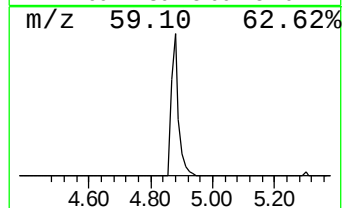
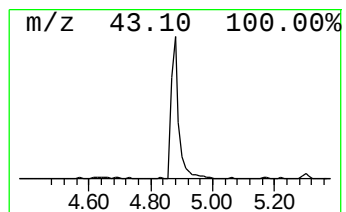
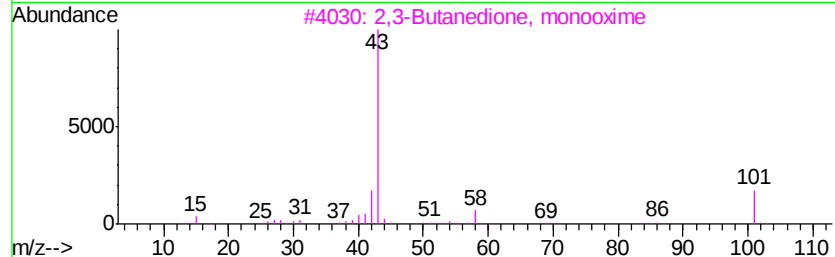
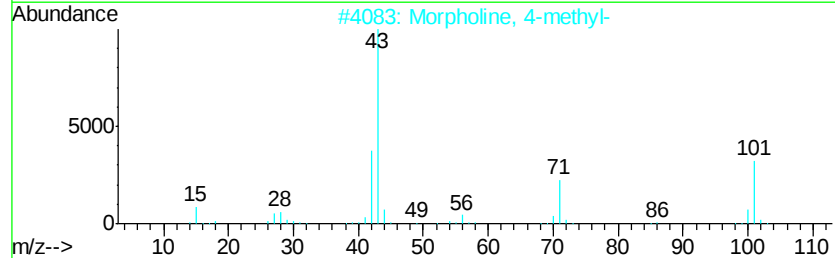
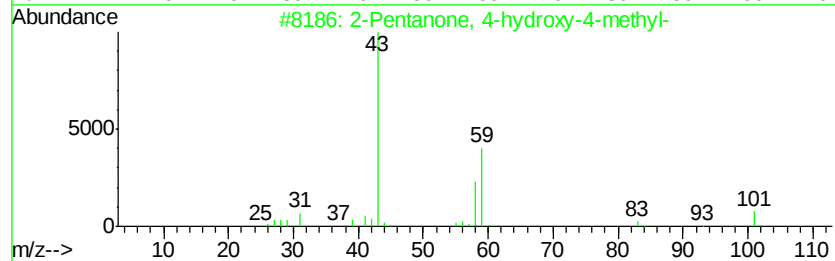
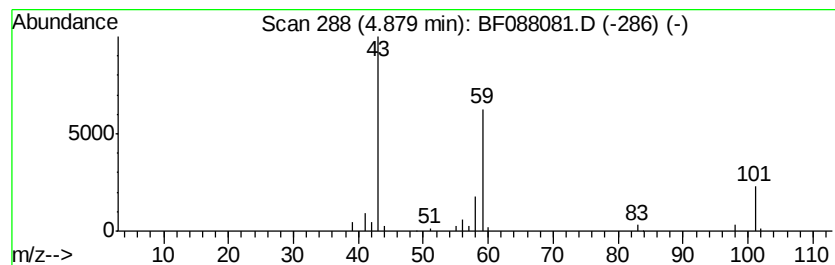
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.88	3.09 ng	101409	1,4-Dichlorobenzene-d4	6.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	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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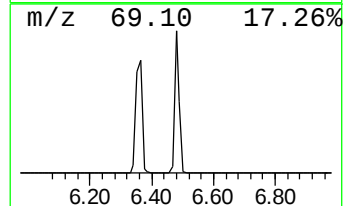
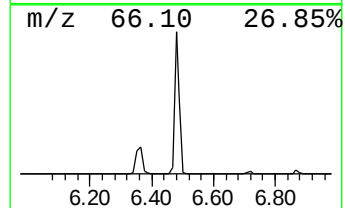
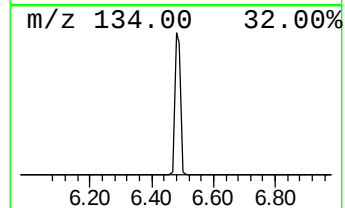
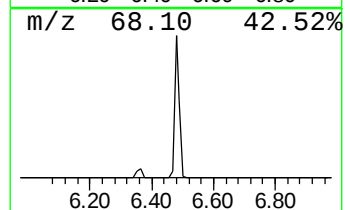
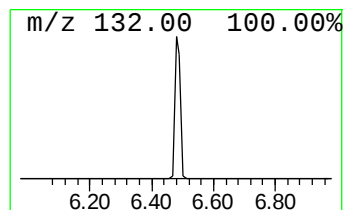
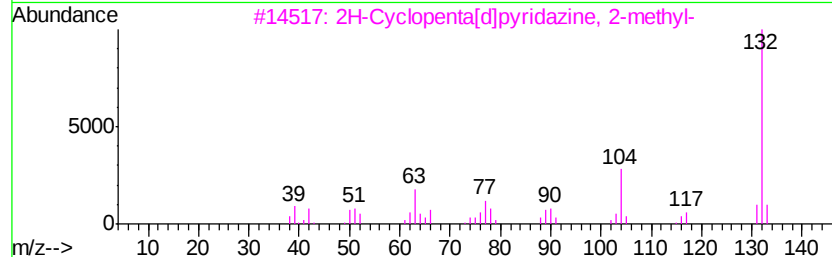
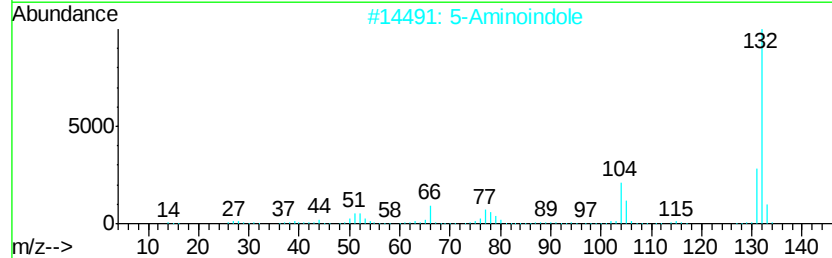
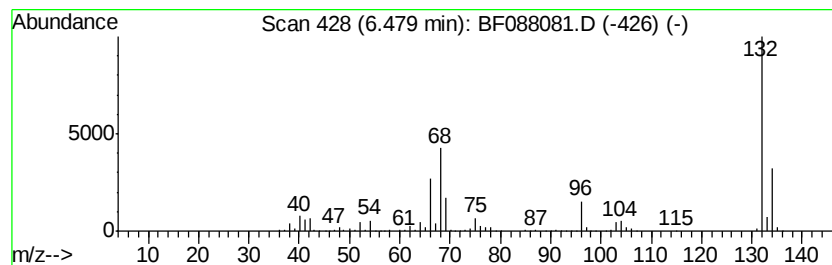
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TIC Library : C:\Database\NIST11.L
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Peak Number 5 unknown6.48 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.48	49.28 ng	1615230	1,4-Dichlorobenzene-d4	6.72

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine			132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole			132	C8H8N2	005192-03-0	12
3	2H-Cyclopenta[d]pyridazine, 2-me...			132	C8H8N2	022291-85-6	9
4	5-Fluoro-2-chloropyrimidine			132	C4H2ClFN2	062802-42-0	9
5	4-Chloro-2-fluoro-pyrimidine			132	C4H2ClFN2	051422-00-5	9



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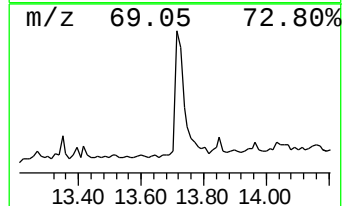
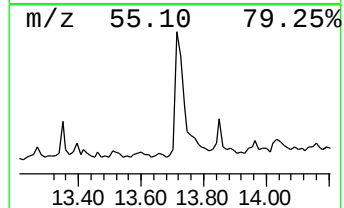
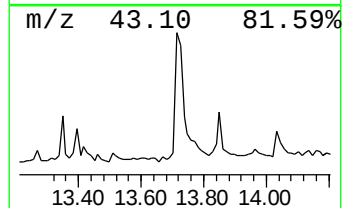
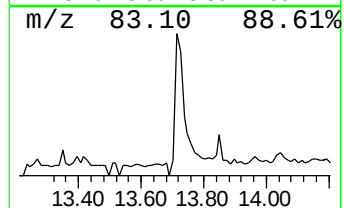
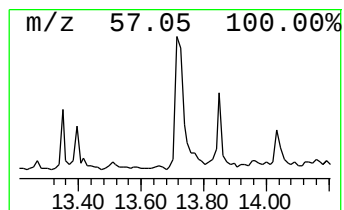
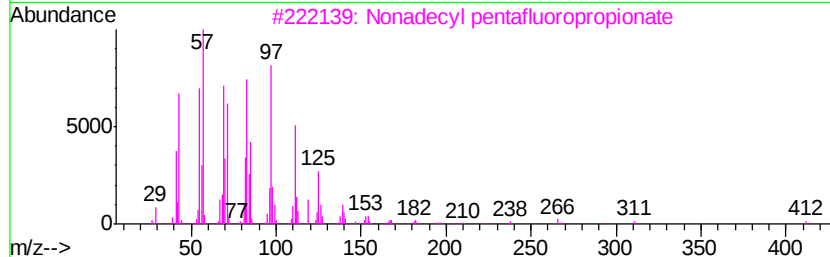
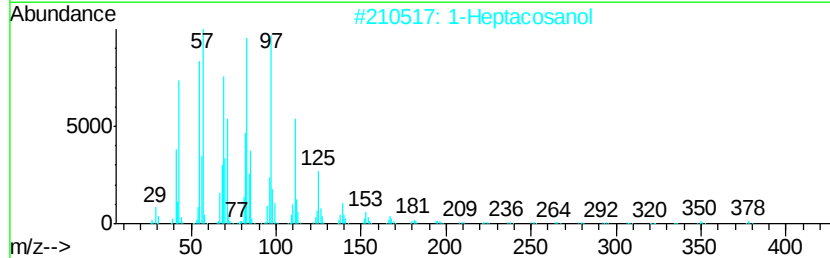
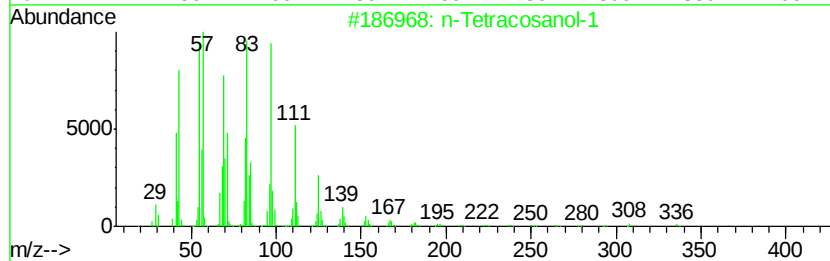
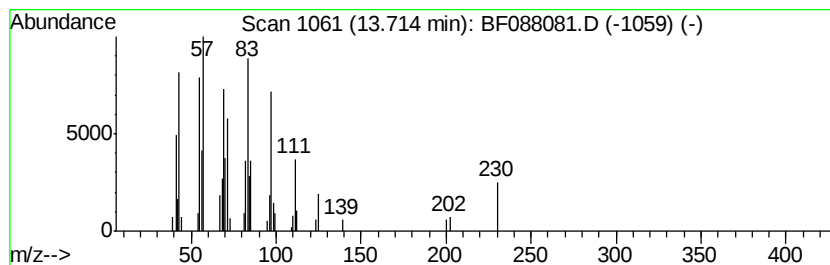
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 n-Tetracosanol-1 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.71	3.01 ng	122000	Chrysene-d12	13.86

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Tetracosanol-1	354	C24H50O	000506-51-4	93
2		1-Heptacosanol	396	C27H56O	002004-39-9	93
3		Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	90
4		1-Docosene	308	C22H44	001599-67-3	90
5		Octacosanol	410	C28H58O	000557-61-9	90



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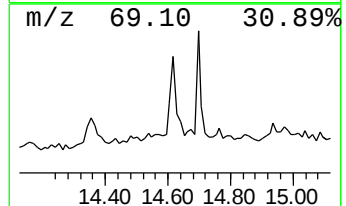
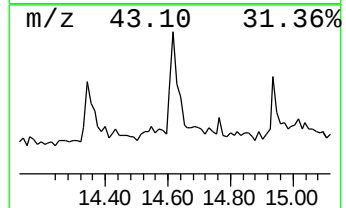
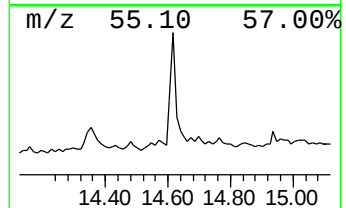
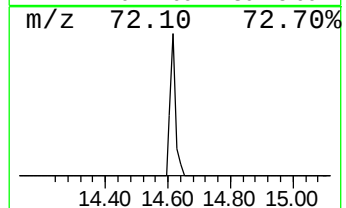
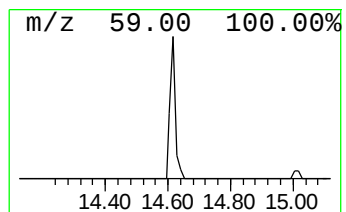
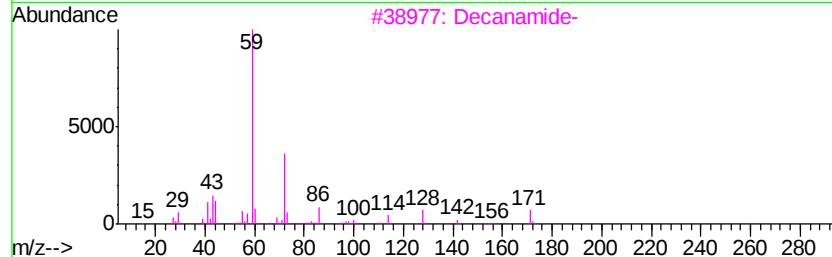
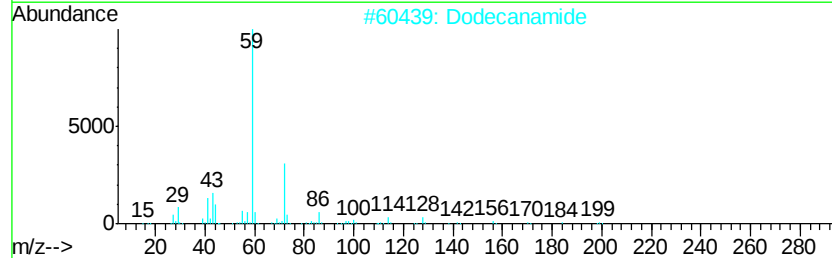
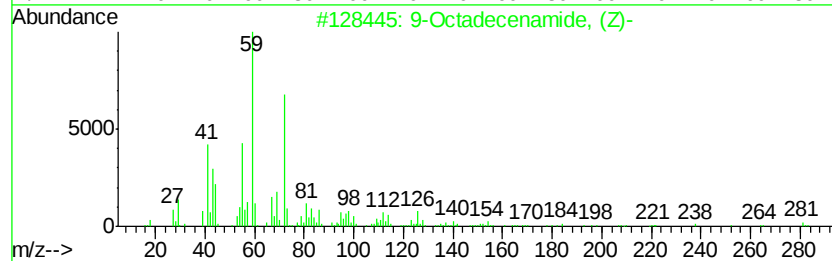
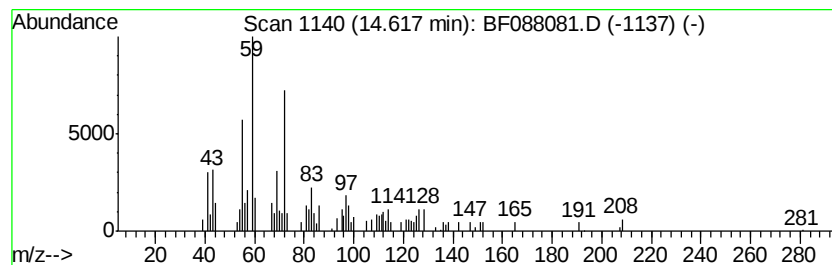
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TIC Library : C:\Database\NIST11.L
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Peak Number 8 9-Octadecenamide, (Z)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.62	2.43 ng	81159	Perylene-d12	15.25

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	86
2		Dodecanamide	199	C12H25NO	001120-16-7	59
3		Decanamide-	171	C10H21NO	002319-29-1	59
4		Pentadecanamide, 15-bromo-	319	C15H30BrNO	1000163-86-1	59
5		Tetradecanamide	227	C14H29NO	000638-58-4	53



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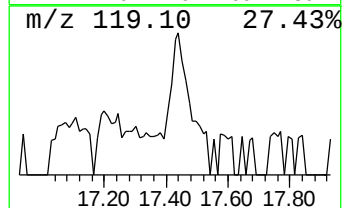
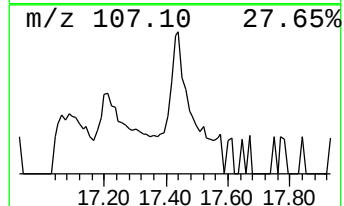
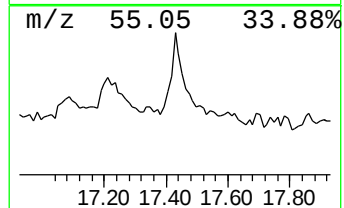
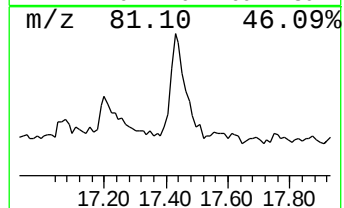
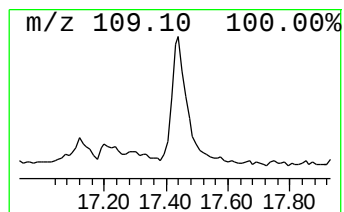
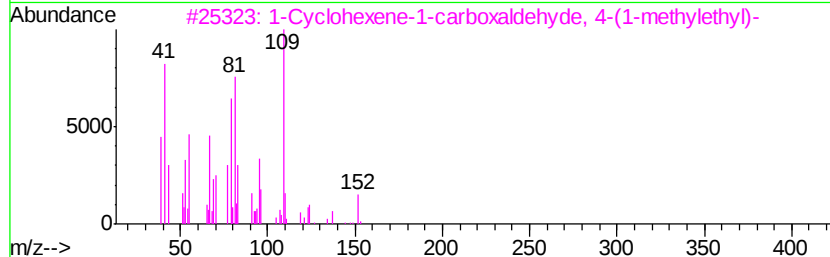
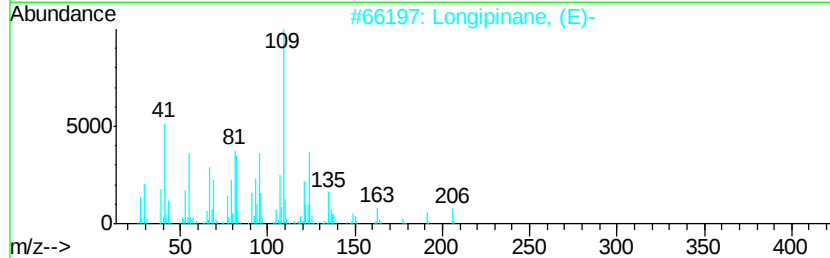
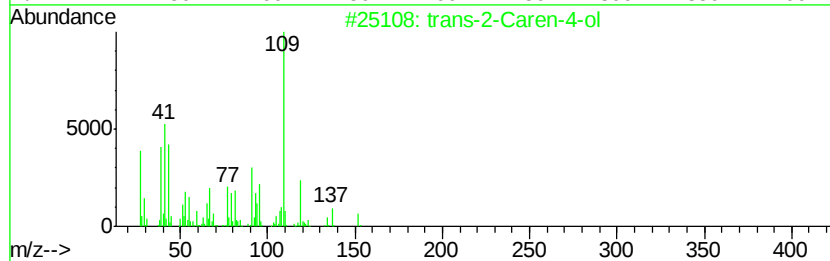
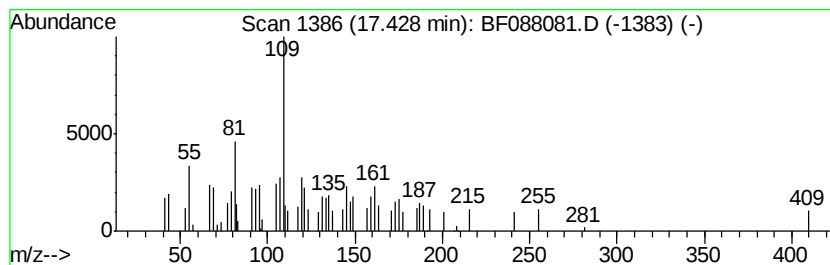
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TIC Library : C:\Database\NIST11.L
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Peak Number 9 unknown17.43 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.43	3.18 ng	106010	Perylene-d12	15.25

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	trans-2-Caren-4-ol	152	C10H16O	004017-82-7	43
2		Longipinane, (E)-	206	C15H26	1000156-14-5	35
3		1-Cyclohexene-1-carboxaldehyde, ...	152	C10H16O	021391-98-0	35
4		2,5,8- Trimethyl-1-nonen-3-yn-5-ol	180	C12H20O	208173-17-5	32
5		trans-3(10)-Caren-2-ol	152	C10H16O	1000151-66-5	32



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.88	3.1	ng	101409	1	6.72	655582	20.0
unknown6.48	6.48	49.3	ng	1615230	1	6.72	655582	20.0
n-Tetracosanol-1	13.71	3.0	ng	122000	5	13.86	809313	20.0
9-Octadecenamide, ...	14.62	2.4	ng	81159	6	15.25	667530	20.0
unknown17.43	17.43	3.2	ng	106010	6	15.25	667530	20.0